Approximation of functions

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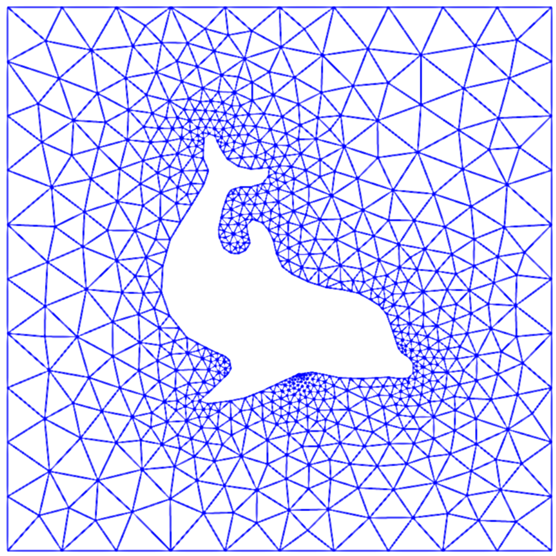
Sep 8, 2015

PRELIMINARY VERSION

Contents

The finite element method is a powerful tool for solving partial differential equations. The method can easily deal with complex geometries and higher-order approximations of the solution. Below is a two-dimensional domain with a non-trivial geometry.



The idea of the finite element method is to divide the domain into triangles (elements) and seek a polynomial approximations to the unknown functions on each triangle. The method glues these piecewise approximations together to find a global solution. Linear and quadratic polynomials over the triangles are particularly popular, because of their mathematical simplicity, but higher-degree polynomials are advantageous to create very computationally efficient methods. The reason for using triangles is that they can easily approximate geometrically complicated domains, but quadrilateral elements and boxes in 3D are also widely used.

Many successful numerical solution methods for differential equations, including the finite element method, aim at approximating the unknown function by a sum

$$u(x) \approx \sum_{i=0}^{N} c_i \psi_i(x), \tag{1}$$

where $\psi_i(x)$ are prescribed functions and $c_0, \ldots, c_N$ are unknown coefficients to be determined. Solution methods for differential equations utilizing (1) must have a *principle* for constructing $N+1$ equations to determine $c_0, \ldots, c_N$. Then there is a *machinery* regarding the actual constructions of the equations for $c_0, \ldots, c_N$, in a particular problem. Finally, there is a *solve* phase for computing the solution $c_0, \ldots, c_N$ of the $N+1$ equations.

Especially in the finite element method, the machinery for constructing the discrete equations to be implemented on a computer is quite comprehensive, with many mathematical and implementational details entering the scene at the same time. From an ease-of-learning perspective it can therefore be wise to follow an idea of Larson and Bengzon [1] and introduce the computational machinery for a trivial equation: $u = f$. Solving this equation with f given and u on the form (1), means that we seek an approximation u to f. This approximation problem has the advantage of introducing most of the finite element toolbox, but without involving demanding topics related to differential equations (e.g., integration by parts, boundary conditions, and coordinate mappings). This is the reason why we shall first become familiar with finite element *approximation* before addressing finite element methods for differential equations.

First, we refresh some linear algebra concepts about approximating vectors in vector spaces. Second, we extend these concepts to approximating functions in function spaces, using the same principles and the same notation. We present examples on approximating functions by global basis functions with support throughout the entire domain. That is, the functions are in general nonzero on the entire domain. Third, we introduce the finite element type of basis functions with local support, meaning that each function is nonzero except in a small part of the domain. We explain all details of the computational algorithms involving such functions. Four types of approximation principles are covered: 1) the least squares method, 2) the L_2 projection or Galerkin method, 3) interpolation or collocation, and 4) the regression method.

1 Approximation of vectors

We shall start with introducing two fundamental methods for determining the coefficients c_i in (1). These methods will be introduce for approximation of vectors. Using vectors in vector spaces to bring across the ideas is believed to appear more intuitive to the reader than starting directly with functions in function spaces. The extension from vectors to functions will be trivial as soon as the fundamental ideas are understood.

The first method of approximation is called the *least squares method* and consists in finding c_i such that the difference $f - u$, measured in a certain norm, is minimized. That is, we aim at finding the best approximation u to f, with the given norm as measure of “distance”. The second method is not as intuitive: we find u such that the error $f - u$ is orthogonal to the space where u lies. This is known as *projection*, or in the context of differential equations, the idea is also well known as *Galerkin's method*. When approximating vectors and functions, the two methods are equivalent, but this is no longer the case when applying the principles to differential equations.

1.1 Approximation of planar vectors

Let $\boldsymbol{f} = (3, 5)$ be a vector in the xy plane and suppose we want to approximate this vector by a vector aligned in the direction of another vector that is restricted to be aligned with some vector (a, b). Figure 1 depicts the situation. This is the simplest approximation problem for vectors. Nevertheless, for many readers it will be wise to refresh some basic linear algebra by consulting a textbook. Exercise 1 suggests specific tasks to regain familiarity with fundamental operations on inner product vector spaces. Familiarity with such operations are assumed in the forthcoming text.

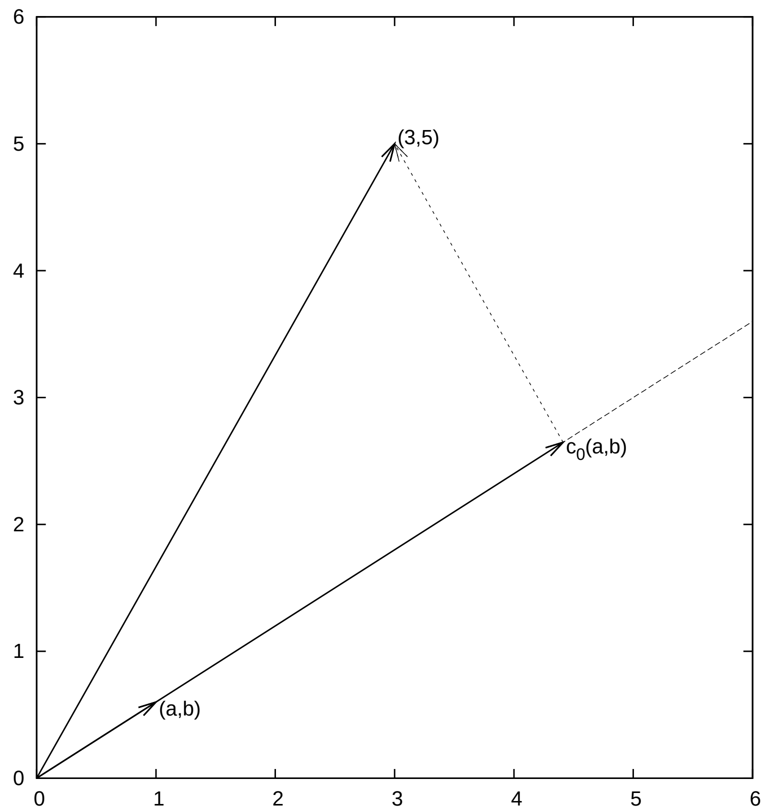


Figure 1: Approximation of a two-dimensional vector in a one-dimensional vector space.

We introduce the vector space V spanned by the vector $\boldsymbol{\psi}_0 = (a, b)$:

$$V = \text{span}\,\{\boldsymbol{\psi}_0\}\,. \tag{2}$$

We say that $\boldsymbol{\psi}_0$ is a *basis vector* in the space V. Our aim is to find the vector $\boldsymbol{u} = c_0\boldsymbol{\psi}_0 \in V$ which best approximates the given vector $\boldsymbol{f} = (3, 5)$. A reasonable criterion for a best approximation could be to minimize the length of the difference between the approximate $\boldsymbol{u}$ and the given $\boldsymbol{f}$. The difference, or error $\boldsymbol{e} = \boldsymbol{f} - \boldsymbol{u}$, has its length given by the *norm*

$$||\boldsymbol{e}|| = (\boldsymbol{e}, \boldsymbol{e})^{\frac{1}{2}},$$

where $(\boldsymbol{e}, \boldsymbol{e})$ is the *inner product* of $\boldsymbol{e}$ and itself. The inner product, also called *scalar product* or *dot product*, of two vectors $\boldsymbol{u} = (u_0, u_1)$ and $\boldsymbol{v} = (v_0, v_1)$ is defined as

$$(\boldsymbol{u}, \boldsymbol{v}) = u_0 v_0 + u_1 v_1 \,. \tag{3}$$

Remark. We should point out that we use the notation $(\cdot, \cdot)$ for two different things: (a, b) for scalar quantities a and b means the vector starting in the origin and ending in the point (a, b), while $(\boldsymbol{u}, \boldsymbol{v})$ with vectors $\boldsymbol{u}$ and $\boldsymbol{v}$ means the inner product of these vectors. Since vectors are here written in boldface font there should be no confusion. We may add that the norm associated with this inner product is the usual Euclidean length of a vector.

The least squares method. We now want to find c_0 such that it minimizes $||\boldsymbol{e}||$. The algebra is simplified if we minimize the square of the norm, $||\boldsymbol{e}||^2 = (\boldsymbol{e}, \boldsymbol{e})$, instead of the norm itself. Define the function

$$E(c_0) = (\boldsymbol{e}, \boldsymbol{e}) = (\boldsymbol{f} - c_0\boldsymbol{\psi}_0, \boldsymbol{f} - c_0\boldsymbol{\psi}_0) \,. \tag{4}$$

We can rewrite the expressions of the right-hand side in a more convenient form for further work:

$$E(c_0) = (\boldsymbol{f}, \boldsymbol{f}) - 2c_0(\boldsymbol{f}, \boldsymbol{\psi}_0) + c_0^2(\boldsymbol{\psi}_0, \boldsymbol{\psi}_0) \,. \tag{5}$$

This rewrite results from using the following fundamental rules for inner product spaces:

$$(\alpha\boldsymbol{u}, \boldsymbol{v}) = \alpha(\boldsymbol{u}, \boldsymbol{v}), \quad \alpha \in \mathbb{R}, \tag{6}$$

$$(\boldsymbol{u} + \boldsymbol{v}, \boldsymbol{w}) = (\boldsymbol{u}, \boldsymbol{w}) + (\boldsymbol{v}, \boldsymbol{w}), \tag{7}$$

$$(\boldsymbol{u}, \boldsymbol{v}) = (\boldsymbol{v}, \boldsymbol{u}) \,. \tag{8}$$

Minimizing $E(c_0)$ implies finding c_0 such that

$$\frac{\partial E}{\partial c_0} = 0 \,.$$

It turns out that E has one unique minimum and no maximum point. Now, when differentiating (5) with respect to c_0, note that none of the inner product expressions depend on c_0, so we simply get

$$\frac{\partial E}{\partial c_0} = -2(\boldsymbol{f}, \boldsymbol{\psi}_0) + 2c_0(\boldsymbol{\psi}_0, \boldsymbol{\psi}_0) \,. \tag{9}$$

Setting the above expression equal to zero and solving for c_0 gives

$$c_0 = \frac{(\boldsymbol{f}, \boldsymbol{\psi}_0)}{(\boldsymbol{\psi}_0, \boldsymbol{\psi}_0)}, \tag{10}$$

which in the present case, with $\boldsymbol{\psi}_0 = (a, b)$, results in

$$c_0 = \frac{3a + 5b}{a^2 + b^2}\,. \tag{11}$$

For later, it is worth mentioning that setting the key equation (9) to zero and ordering the terms lead to

$$(\boldsymbol{f} - c0\boldsymbol{\psi}_0, \boldsymbol{\psi}_0) = 0,$$

or

$$(\boldsymbol{e}, \boldsymbol{\psi}_0) = 0\,. \tag{12}$$

This implication of minimizing E is an important result that we shall make much use of.

The projection method. We shall now show that minimizing $||\boldsymbol{e}||^2$ implies that $\boldsymbol{e}$ is orthogonal to *any* vector $\boldsymbol{v}$ in the space V. This result is visually quite clear from Figure 1 (think of other vectors along the line (a, b): all of them will lead to a larger distance between the approximation and $\boldsymbol{f}$). The see mathematically that $\boldsymbol{e}$ is orthogonal to any vector $\boldsymbol{v}$ in the space V, we express any $\boldsymbol{v} \in V$ as $\boldsymbol{v} = s\boldsymbol{\psi}_0$ for any scalar parameter s (recall that two vectors are orthogonal when their inner product vanishes). Then we calculate the inner product

$$\begin{aligned}
(\boldsymbol{e}, s\boldsymbol{\psi}_0) &= (\boldsymbol{f} - c_0\boldsymbol{\psi}_0, s\boldsymbol{\psi}_0)\\
&= (\boldsymbol{f}, s\boldsymbol{\psi}_0) - (c_0\boldsymbol{\psi}_0, s\boldsymbol{\psi}_0)\\
&= s(\boldsymbol{f}, \boldsymbol{\psi}_0) - sc_0(\boldsymbol{\psi}_0, \boldsymbol{\psi}_0)\\
&= s(\boldsymbol{f}, \boldsymbol{\psi}_0) - s\frac{(\boldsymbol{f}, \boldsymbol{\psi}_0)}{(\boldsymbol{\psi}_0, \boldsymbol{\psi}_0)}(\boldsymbol{\psi}_0, \boldsymbol{\psi}_0)\\
&= s\left((\boldsymbol{f}, \boldsymbol{\psi}_0) - (\boldsymbol{f}, \boldsymbol{\psi}_0)\right)\\
&= 0\,.
\end{aligned}$$

Therefore, instead of minimizing the square of the norm, we could demand that $\boldsymbol{e}$ is orthogonal to any vector in V, which in our present simple case amounts to a single vector only. This method is known as *projection*. (The approach can also be referred to as a Galerkin method as explained at the end of Section 1.2.)

Mathematically, the projection method is stated by the equation

$$(\boldsymbol{e}, \boldsymbol{v}) = 0, \quad \forall \boldsymbol{v} \in V\,. \tag{13}$$

An arbitrary $\boldsymbol{v} \in V$ can be expressed as $s\boldsymbol{\psi}_0$, $s \in \mathbb{R}$, and therefore (13) implies

$$(\boldsymbol{e}, s\boldsymbol{\psi}_0) = s(\boldsymbol{e}, \boldsymbol{\psi}_0) = 0,$$

which means that the error must be orthogonal to the basis vector in the space V:

$$(\boldsymbol{e}, \boldsymbol{\psi}_0) = 0 \quad \text{or} \quad (\boldsymbol{f} - c_0\boldsymbol{\psi}_0, \boldsymbol{\psi}_0) = 0,$$

which is what we found in (12) from the least squares computations.

1.2 Approximation of general vectors

Let us generalize the vector approximation from the previous section to vectors in spaces with arbitrary dimension. Given some vector $\boldsymbol{f}$, we want to find the best approximation to this vector in the space

$$V = \text{span}\,\{\boldsymbol{\psi}_0, \ldots, \boldsymbol{\psi}_N\}\,.$$

We assume that the space has dimension $N+1$ and that *basis vectors* $\boldsymbol{\psi}_0, \ldots, \boldsymbol{\psi}_N$ are linearly independent so that none of them are redundant. Any vector $\boldsymbol{u} \in V$ can then be written as a linear combination of the basis vectors, i.e.,

$$\boldsymbol{u} = \sum_{j=0}^{N} c_j\boldsymbol{\psi}_j,$$

where $c_j \in \mathbb{R}$ are scalar coefficients to be determined.

The least squares method. Now we want to find $c_0, \ldots, c_N$, such that $\boldsymbol{u}$ is the best approximation to $\boldsymbol{f}$ in the sense that the distance (error) $\boldsymbol{e} = \boldsymbol{f} - \boldsymbol{u}$ is minimized. Again, we define the squared distance as a function of the free parameters $c_0, \ldots, c_N$,

$$\begin{aligned} E(c_0, \ldots, c_N) &= (\boldsymbol{e}, \boldsymbol{e}) = (\boldsymbol{f} - \sum_j c_j\boldsymbol{\psi}_j, \boldsymbol{f} - \sum_j c_j\boldsymbol{\psi}_j) \\ &= (\boldsymbol{f}, \boldsymbol{f}) - 2\sum_{j=0}^{N} c_j(\boldsymbol{f}, \boldsymbol{\psi}_j) + \sum_{p=0}^{N}\sum_{q=0}^{N} c_p c_q(\boldsymbol{\psi}_p, \boldsymbol{\psi}_q)\,. \end{aligned} \tag{14}$$

Minimizing this E with respect to the independent variables $c_0, \ldots, c_N$ is obtained by requiring

$$\frac{\partial E}{\partial c_i} = 0, \quad i = 0, \ldots, N\,.$$

The first term in (14) is independent of c_i, so its derivative vanishes. The second term in (14) is differentiated as follows:

$$\frac{\partial}{\partial c_i} 2\sum_{j=0}^{N} c_j(\boldsymbol{f},\boldsymbol{\psi}_j) = 2(\boldsymbol{f},\boldsymbol{\psi}_i), \tag{15}$$

since the expression to be differentiated is a sum and only one term, $c_i(\boldsymbol{f},\boldsymbol{\psi}_i)$, contains c_i (this term is linear in c_i). To understand this differentiation in detail, write out the sum specifically for, e.g, $N=3$ and $i=1$.

The last term in (14) is more tedious to differentiate. It can be wise to write out the double sum for $N=1$ and perform differentiation with respect to c_0 and c_1 to see the structure of the expression. Thereafter, one can generalize to an arbitrary N and observe that

$$\frac{\partial}{\partial c_i} c_p c_q = \begin{cases} 0, & \text{if } p \neq i \text{ and } q \neq i,\\ c_q, & \text{if } p = i \text{ and } q \neq i,\\ c_p, & \text{if } p \neq i \text{ and } q = i,\\ 2c_i, & \text{if } p = q = i\,. \end{cases} \tag{16}$$

Then

$$\frac{\partial}{\partial c_i} \sum_{p=0}^{N}\sum_{q=0}^{N} c_p c_q(\boldsymbol{\psi}_p,\boldsymbol{\psi}_q) = \sum_{p=0,p\neq i}^{N} c_p(\boldsymbol{\psi}_p,\boldsymbol{\psi}_i) + \sum_{q=0,q\neq i}^{N} c_q(\boldsymbol{\psi}_i,\boldsymbol{\psi}_q) + 2c_i(\boldsymbol{\psi}_i,\boldsymbol{\psi}_i)\,.$$

Since each of the two sums is missing the term $c_i(\boldsymbol{\psi}_i,\boldsymbol{\psi}_i)$, we may split the very last term in two, to get exactly that "missing" term for each sum. This idea allows us to write

$$\frac{\partial}{\partial c_i} \sum_{p=0}^{N}\sum_{q=0}^{N} c_p c_q(\boldsymbol{\psi}_p,\boldsymbol{\psi}_q) = 2\sum_{j=0}^{N} c_i(\boldsymbol{\psi}_j,\boldsymbol{\psi}_i)\,. \tag{17}$$

It then follows that setting

$$\frac{\partial E}{\partial c_i} = 0, \quad i = 0,\ldots,N,$$

implies

$$-2(\boldsymbol{f},\boldsymbol{\psi}_i) + 2\sum_{j=0}^{N} c_i(\boldsymbol{\psi}_j,\boldsymbol{\psi}_i) = 0, \quad i = 0,\ldots,N\,.$$

Moving the first term to the right-hand side shows that the equation is actually a *linear system* for the unknown parameters $c_0,\ldots,c_N$:

$$\sum_{j=0}^{N} A_{i,j} c_j = b_i, \quad i = 0,\ldots,N, \tag{18}$$

where

$$
\begin{aligned}
A_{i,j} &= (\boldsymbol{\psi}_i, \boldsymbol{\psi}_j), &(19)\\
b_i &= (\boldsymbol{\psi}_i, \boldsymbol{f})\,. &(20)
\end{aligned}
$$

We have changed the order of the two vectors in the inner product according to (1.1):

$$A_{i,j} = (\boldsymbol{\psi}_j, \boldsymbol{\psi}_i) = (\boldsymbol{\psi}_i, \boldsymbol{\psi}_j),$$

simply because the sequence i-j looks more aesthetic.

The Galerkin or projection method. In analogy with the "one-dimensional" example in Section 1.1, it holds also here in the general case that minimizing the distance (error) $\boldsymbol{e}$ is equivalent to demanding that $\boldsymbol{e}$ is orthogonal to all $\boldsymbol{v} \in V$:

$$(\boldsymbol{e}, \boldsymbol{v}) = 0, \quad \forall \boldsymbol{v} \in V\,. \tag{21}$$

Since any $\boldsymbol{v} \in V$ can be written as $\boldsymbol{v} = \sum_{i=0}^{N} c_i \boldsymbol{\psi}_i$, the statement (21) is equivalent to saying that

$$(\boldsymbol{e}, \sum_{i=0}^{N} c_i \boldsymbol{\psi}_i) = 0,$$

for any choice of coefficients $c_0, \ldots, c_N$. The latter equation can be rewritten as

$$\sum_{i=0}^{N} c_i (\boldsymbol{e}, \boldsymbol{\psi}_i) = 0\,.$$

If this is to hold for arbitrary values of $c_0, \ldots, c_N$ we must require that each term in the sum vanishes, which means that

$$(\boldsymbol{e}, \boldsymbol{\psi}_i) = 0, \quad i = 0, \ldots, N\,. \tag{22}$$

These $N + 1$ equations result in the same linear system as (18):

$$(\boldsymbol{f} - \sum_{j=0}^{N} c_j \boldsymbol{\psi}_j, \boldsymbol{\psi}_i) = (\boldsymbol{f}, \boldsymbol{\psi}_i) - \sum_{j=0}^{N} (\boldsymbol{\psi}_i, \boldsymbol{\psi}_j) c_j = 0,$$

and hence

$$\sum_{j=0}^{N} (\boldsymbol{\psi}_i, \boldsymbol{\psi}_j) c_j = (\boldsymbol{f}, \boldsymbol{\psi}_i), \quad i = 0, \ldots, N\,.$$

So, instead of differentiating the $E(c_0, \ldots, c_N)$ function, we could simply use (21) as the principle for determining $c_0, \ldots, c_N$, resulting in the $N + 1$ equations (22).

The names *least squares method* or *least squares approximation* are natural since the calculations consists of minimizing $||\boldsymbol{e}||^2$, and $||\boldsymbol{e}||^2$ is a sum of squares of differences between the components in $\boldsymbol{f}$ and $\boldsymbol{u}$. We find $\boldsymbol{u}$ such that this sum of squares is minimized.

The principle (21), or the equivalent form (22), is known as *projection*. Almost the same mathematical idea was used by the Russian mathematician Boris Galerkin to solve differential equations, resulting in what is widely known as *Galerkin's method*.

2 Approximation of functions

Let V be a function space spanned by a set of *basis functions* $\psi_0, \ldots, \psi_N$,

$$V = \operatorname{span}\{\psi_0, \ldots, \psi_N\},$$

such that any function $u \in V$ can be written as a linear combination of the basis functions:

$$u = \sum_{j\in\mathcal{I}_s} c_j\psi_j\,. \tag{23}$$

The index set $\mathcal{I}_s$ is defined as $\mathcal{I}_s = \{0, \ldots, N\}$ and is from now on used both for compact notation and for flexibility in the numbering of elements in sequences.

For now, in this introduction, we shall look at functions of a single variable x: $u = u(x)$, $\psi_j = \psi_j(x)$, $j \in \mathcal{I}_s$. Later, we will almost trivially extend the mathematical details to functions of two- or three-dimensional physical spaces. The approximation (23) is typically used to discretize a problem in space. Other methods, most notably finite differences, are common for time discretization, although the form (23) can be used in time as well.

2.1 The least squares method

Given a function $f(x)$, how can we determine its best approximation $u(x) \in V$? A natural starting point is to apply the same reasoning as we did for vectors in Section 1.2. That is, we minimize the distance between u and f. However, this requires a norm for measuring distances, and a norm is most conveniently defined through an inner product. Viewing a function as a vector of infinitely many point values, one for each value of x, the inner product of two arbitrary functions $f(x)$ and $g(x)$ could intuitively be defined as the usual summation of pairwise "components" (values), with summation replaced by integration:

$$(f, g) = \int f(x)g(x)\, \mathrm{d}x\,.$$

To fix the integration domain, we let $f(x)$ and $\psi_i(x)$ be defined for a domain $\Omega \subset \mathbb{R}$. The inner product of two functions $f(x)$ and $g(x)$ is then

$$(f,g) = \int_\Omega f(x)g(x)\,\mathrm{d}x\,. \tag{24}$$

The distance between f and any function $u \in V$ is simply $f-u$, and the squared norm of this distance is

$$E = (f(x) - \sum_{j\in\mathcal{I}_s} c_j\psi_j(x), f(x) - \sum_{j\in\mathcal{I}_s} c_j\psi_j(x))\,. \tag{25}$$

Note the analogy with (14): the given function f plays the role of the given vector $\boldsymbol{f}$, and the basis function ψ_i plays the role of the basis vector $\boldsymbol{\psi}_i$. We can rewrite (25), through similar steps as used for the result (14), leading to

$$E(c_i,\ldots,c_N) = (f,f) - 2\sum_{j\in\mathcal{I}_s} c_j(f,\psi_i) + \sum_{p\in\mathcal{I}_s}\sum_{q\in\mathcal{I}_s} c_pc_q(\psi_p,\psi_q)\,. \tag{26}$$

Minimizing this function of $N+1$ scalar variables $\{c_i\}_{i\in\mathcal{I}_s}$, requires differentiation with respect to c_i, for all $i\in\mathcal{I}_s$. The resulting equations are very similar to those we had in the vector case, and we hence end up with a linear system of the form (18), with basically the same expressions:

$$A_{i,j} = (\psi_i,\psi_j), \tag{27}$$

$$b_i = (f,\psi_i)\,. \tag{28}$$

2.2 The projection (or Galerkin) method

As in Section 1.2, the minimization of (e,e) is equivalent to

$$(e,v) = 0,\quad \forall v\in V\,. \tag{29}$$

This is known as a projection of a function f onto the subspace V. We may also call it a Galerkin method for approximating functions. Using the same reasoning as in (21)-(22), it follows that (29) is equivalent to

$$(e,\psi_i) = 0,\quad i\in\mathcal{I}_s\,. \tag{30}$$

Inserting $e = f-u$ in this equation and ordering terms, as in the multi-dimensional vector case, we end up with a linear system with a coefficient matrix (27) and right-hand side vector (28).

Whether we work with vectors in the plane, general vectors, or functions in function spaces, the least squares principle and the projection or Galerkin method are equivalent.

2.3 Example: linear approximation

Let us apply the theory in the previous section to a simple problem: given a parabola $f(x) = 10(x-1)^2 - 1$ for $x \in \Omega = [1,2]$, find the best approximation $u(x)$ in the space of all linear functions:

$$V = \text{span}\,\{1, x\}\,.$$

With our notation, $\psi_0(x) = 1$, $\psi_1(x) = x$, and $N = 1$. We seek

$$u = c_0\psi_0(x) + c_1\psi_1(x) = c_0 + c_1 x,$$

where c_0 and c_1 are found by solving a 2×2 the linear system. The coefficient matrix has elements

$$A_{0,0} = (\psi_0, \psi_0) = \int_1^2 1\cdot 1\ \mathrm{d}x = 1, \tag{31}$$

$$A_{0,1} = (\psi_0, \psi_1) = \int_1^2 1\cdot x\ \mathrm{d}x = 3/2, \tag{32}$$

$$A_{1,0} = A_{0,1} = 3/2, \tag{33}$$

$$A_{1,1} = (\psi_1, \psi_1) = \int_1^2 x\cdot x\ \mathrm{d}x = 7/3\,. \tag{34}$$

The corresponding right-hand side is

$$b_1 = (f, \psi_0) = \int_1^2 (10(x-1)^2 - 1)\cdot 1\ \mathrm{d}x = 7/3, \tag{35}$$

$$b_2 = (f, \psi_1) = \int_1^2 (10(x-1)^2 - 1)\cdot x\ \mathrm{d}x = 13/3\,. \tag{36}$$

Solving the linear system results in

$$c_0 = -38/3, \quad c_1 = 10, \tag{37}$$

and consequently

$$u(x) = 10x - \frac{38}{3}\,. \tag{38}$$

Figure 2 displays the parabola and its best approximation in the space of all linear functions.

2.4 Implementation of the least squares method

Symbolic integration. The linear system can be computed either symbolically or numerically (a numerical integration rule is needed in the latter case). Let us first compute the system and its solution symbolically, i.e., using classical

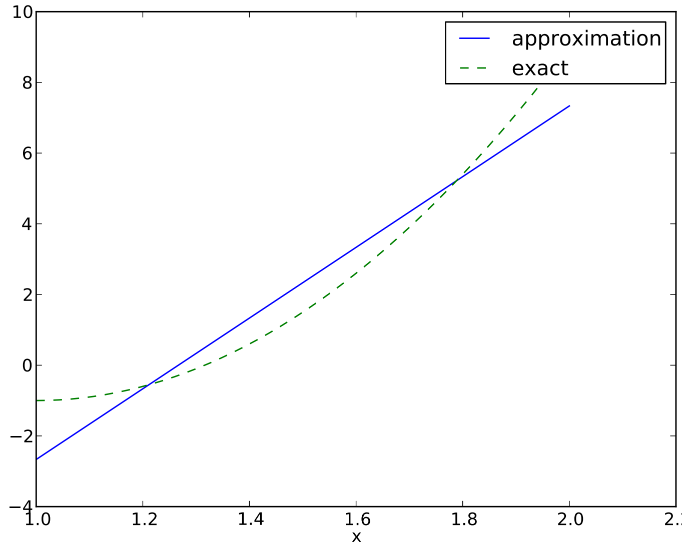


Figure 2: Best approximation of a parabola by a straight line.

"pen and paper" mathematics with symbols. The Python package `sympy` can greatly help with this type of mathematics, and will therefore be frequently used in this text. Some basic familiarity with `sympy` is assumed, typically `symbols`, `integrate`, `diff`, `expand`, and `simplify`. Much can be learned by studying the many applications of `sympy` that will be presented.

Below is a function for symbolic computation of the linear system, where $f(x)$ is given as a `sympy` expression `f` involving the symbol `x`, `psi` is a list of expressions for $\{\psi_i\}_{i\in\mathcal{I}_s}$, and `Omega` is a 2-tuple/list holding the limits of the domain Ω:

```
import sympy as sym

def least_squares(f, psi, Omega):
    N = len(psi) - 1
    A = sym.zeros((N+1, N+1))
    b = sym.zeros((N+1, 1))
    x = sym.Symbol('x')
    for i in range(N+1):
        for j in range(i, N+1):
            A[i,j] = sym.integrate(psi[i]*psi[j],
                                   (x, Omega[0], Omega[1]))
            A[j,i] = A[i,j]
        b[i,0] = sym.integrate(psi[i]*f, (x, Omega[0], Omega[1]))
    c = A.LUsolve(b)
    # Note: c is a sympy Matrix object, solution is in c[:,0]
    u = 0
    for i in range(len(psi)):
```

```
        u += c[i,0]*psi[i]
    return u, c
```

Observe that we exploit the symmetry of the coefficient matrix: only the upper triangular part is computed. Symbolic integration, also in `sympy`, is often time consuming, and (roughly) halving the work has noticeable effect on the waiting time for the computations to finish.

Fall back on numerical integration. Obviously, `sympy` may fail to successfully integrate $\int_\Omega \psi_i\psi_j \,\mathrm{d}x$, and especially $\int_\Omega f\psi_i \,\mathrm{d}x$, symbolically. Therefore, we should extend the `least_squares` function such that it falls back on numerical integration if the symbolic integration is unsuccessful. In the latter case, the returned value from `sympy`'s `integrate` function is an object of type `Integral`. We can test on this type and utilize the `mpmath` module in `sympy` to perform numerical integration of high precision. Even when `sympy` manages to integrate symbolically, it can take an undesirable long time. We therefore include an argument `symbolic` that governs whether or not to try symbolic integration. Here is a complete and improved version of the previous function `least_squares`:

```
def least_squares(f, psi, Omega, symbolic=True):
    N = len(psi) - 1
    A = sym.zeros((N+1, N+1))
    b = sym.zeros((N+1, 1))
    x = sym.Symbol('x')
    for i in range(N+1):
        for j in range(i, N+1):
            integrand = psi[i]*psi[j]
            if symbolic:
                I = sym.integrate(integrand, (x, Omega[0], Omega[1]))
            if not symbolic or isinstance(I, sym.Integral):
                # Could not integrate symbolically,
                # fall back on numerical integration
                integrand = sym.lambdify([x], integrand)
                I = sym.mpmath.quad(integrand, [Omega[0], Omega[1]])
            A[i,j] = A[j,i] = I

        integrand = psi[i]*f
        if symbolic:
            I = sym.integrate(integrand, (x, Omega[0], Omega[1]))
        if not symbolic or isinstance(I, sym.Integral):
            integrand = sym.lambdify([x], integrand)
            I = sym.mpmath.quad(integrand, [Omega[0], Omega[1]])
        b[i,0] = I
    c = A.LUsolve(b)  # symbolic solve
    # c is a sympy Matrix object, numbers are in c[i,0]
    c = [sym.simplify(c[i,0]) for i in range(c.shape[0])]
    u = sum(c[i]*psi[i] for i in range(len(psi)))
    return u, c
```

The function is found in the file `approx1D.py`.

Plotting the approximation. Comparing the given $f(x)$ and the approximate $u(x)$ visually is done by the following function, which utilizes `sympy`'s `lambdify` tool to convert a `sympy` expression to a Python function for numerical computations:

```
def comparison_plot(f, u, Omega, filename='tmp.pdf'):
    x = sym.Symbol('x')
    f = sym.lambdify([x], f, modules="numpy")
    u = sym.lambdify([x], u, modules="numpy")
    resolution = 401  # no of points in plot
    xcoor  = linspace(Omega[0], Omega[1], resolution)
    exact  = f(xcoor)
    approx = u(xcoor)
    plot(xcoor, approx)
    hold('on')
    plot(xcoor, exact)
    legend(['approximation', 'exact'])
    savefig(filename)
```

The `modules='numpy'` argument to `lambdify` is important if there are mathematical functions, such as `sin` or `exp` in the symbolic expressions in `f` or `u`, and these mathematical functions are to be used with vector arguments, like `xcoor` above.

Both the `least_squares` and `comparison_plot` functions are found in the file `approx1D.py`. The `comparison_plot` function in this file is more advanced and flexible than the simplistic version shown above. The file `ex_approx1D.py` applies the `approx1D` module to accomplish the forthcoming examples.

2.5 Perfect approximation

Let us use the code above to recompute the problem from Section 2.3 where we want to approximate a parabola. What happens if we add an element x^2 to the basis and test what the best approximation is if V is the space of all parabolic functions? The answer is quickly found by running

```
>>> from approx1D import *
>>> x = sym.Symbol('x')
>>> f = 10*(x-1)**2-1
>>> u, c = least_squares(f=f, psi=[1, x, x**2], Omega=[1, 2])
>>> print u
10*x**2 - 20*x + 9
>>> print sym.expand(f)
10*x**2 - 20*x + 9
```

Now, what if we use $\psi_i(x) = x^i$ for $i = 0, 1, \ldots, N = 40$? The output from `least_squares` gives $c_i = 0$ for $i > 2$, which means that the method finds the perfect approximation.

In fact, we have a general result that if $f \in V$, the least squares and projection/Galerkin methods compute the exact solution $u = f$. The proof is straightforward: if $f \in V$, f can be expanded in terms of the basis functions, $f = \sum_{j\in\mathcal{I}_s} d_j\psi_j$, for some coefficients $\{d_j\}_{j\in\mathcal{I}_s}$, and the right-hand side then has entries

$$b_i = (f, \psi_i) = \sum_{j\in\mathcal{I}_s} d_j(\psi_j, \psi_i) = \sum_{j\in\mathcal{I}_s} d_j A_{i,j}\,.$$

The linear system $\sum_j A_{i,j}c_j = b_i$, $i \in \mathcal{I}_s$, is then

$$\sum_{j\in\mathcal{I}_s} c_j A_{i,j} = \sum_{j\in\mathcal{I}_s} d_j A_{i,j}, \quad i \in \mathcal{I}_s,$$

which implies that $c_i = d_i$ for $i \in \mathcal{I}_s$.

2.6 Ill-conditioning

The computational example in Section 2.5 applies the `least_squares` function which invokes symbolic methods to calculate and solve the linear system. The correct solution $c_0 = 9, c_1 = -20, c_2 = 10, c_i = 0$ for $i \geq 3$ is perfectly recovered.

Suppose we convert the matrix and right-hand side to floating-point arrays and then solve the system using finite-precision arithmetics, which is what one will (almost) always do in real life. This time we get astonishing results! Up to about $N = 7$ we get a solution that is reasonably close to the exact one. Increasing N shows that seriously wrong coefficients are computed. Below is a table showing the solution of the linear system arising from approximating a parabola by functions on the form $u(x) = c_0 + c_1x + c_2x^2 + \cdots + c_{10}x^{10}$. Analytically, we know that $c_j = 0$ for $j > 2$, but numerically we may get $c_j \neq 0$ for $j > 2$.

exact	`sympy`	`numpy32`	`numpy64`
9	9.62	5.57	8.98
-20	-23.39	-7.65	-19.93
10	17.74	-4.50	9.96
0	-9.19	4.13	-0.26
0	5.25	2.99	0.72
0	0.18	-1.21	-0.93
0	-2.48	-0.41	0.73
0	1.81	-0.013	-0.36
0	-0.66	0.08	0.11
0	0.12	0.04	-0.02
0	-0.001	-0.02	0.002

The exact value of c_j, $j = 0, 1, \ldots, 10$, appears in the first column while the other columns correspond to results obtained by three different methods:

- Column 2: The matrix and vector are converted to the data structure `sympy.mpmath.fp.matrix` and the `sympy.mpmath.fp.lu_solve` function is used to solve the system.
- Column 3: The matrix and vector are converted to `numpy` arrays with data type `numpy.float32` (single precision floating-point number) and solved by the `numpy.linalg.solve` function.
- Column 4: As column 3, but the data type is `numpy.float64` (double precision floating-point number).

We see from the numbers in the table that double precision performs much better than single precision. Nevertheless, when plotting all these solutions the curves cannot be visually distinguished (!). This means that the approximations look perfect, despite the partially very wrong values of the coefficients.

Increasing N to 12 makes the numerical solver in `numpy` abort with the message: "matrix is numerically singular". A matrix has to be non-singular to be invertible, which is a requirement when solving a linear system. Already when the matrix is close to singular, it is *ill-conditioned*, which here implies that the numerical solution algorithms are sensitive to round-off errors and may produce (very) inaccurate results.

The reason why the coefficient matrix is nearly singular and ill-conditioned is that our basis functions $\psi_i(x) = x^i$ are nearly linearly dependent for large i. That is, x^i and x^{i+1} are very close for i not very small. This phenomenon is illustrated in Figure 3. There are 15 lines in this figure, but only half of them are visually distinguishable. Almost linearly dependent basis functions give rise to an ill-conditioned and almost singular matrix. This fact can be illustrated by computing the determinant, which is indeed very close to zero (recall that a zero determinant implies a singular and non-invertible matrix): 10^{-65} for $N = 10$ and 10^{-92} for $N = 12$. Already for $N = 28$ the numerical determinant computation returns a plain zero.

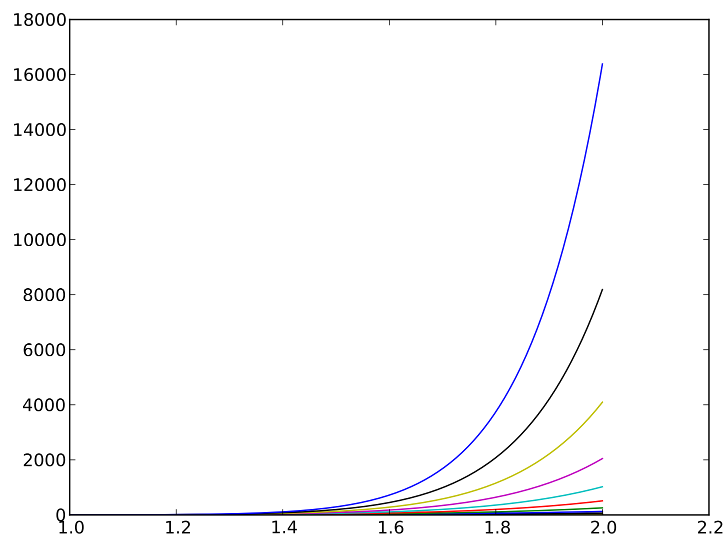


Figure 3: The 15 first basis functions x^i, $i = 0, \ldots, 14$.

On the other hand, the double precision `numpy` solver does run for $N = 100$, resulting in answers that are not significantly worse than those in the table above, and large powers are associated with small coefficients (e.g., $c_j < 10^{-2}$ for $10 \leq j \leq 20$ and $c < 10^{-5}$ for $j > 20$). Even for $N = 100$ the approximation still lies on top of the exact curve in a plot (!).

The conclusion is that visual inspection of the quality of the approximation may not uncover fundamental numerical problems with the computations. However, numerical analysts have studied approximations and ill-conditioning for decades, and it is well known that the basis $\{1, x, x^2, x^3, \ldots, \}$ is a bad basis. The best basis from a matrix conditioning point of view is to have orthogonal functions such that $(\psi_i, \psi_j) = 0$ for $i \neq j$. There are many known sets of orthogonal polynomials and other functions. The functions used in the finite element methods are almost orthogonal, and this property helps to avoid problems with solving matrix systems. Almost orthogonal is helpful, but not enough when it comes to partial differential equations, and ill-conditioning of the coefficient matrix is a theme when solving large-scale matrix systems arising from finite element discretizations.

2.7 Fourier series

A set of sine functions is widely used for approximating functions (the sines are also orthogonal as explained more in Section 2.6). Let us take

$$V = \text{span}\{\sin \pi x, \sin 2\pi x, \ldots, \sin(N+1)\pi x\}.$$

That is,

$$\psi_i(x) = \sin((i+1)\pi x), \quad i \in \mathcal{I}_s.$$

An approximation to the parabola $f(x) = 10(x-1)^2 - 1$ for $x \in \Omega = [1, 2]$ from Section 2.3 can then be computed by the `least_squares` function from Section 2.4:

```
N = 3
import sympy as sym
x = sym.Symbol('x')
psi = [sym.sin(sym.pi*(i+1)*x) for i in range(N+1)]
f = 10*(x-1)**2 - 1
Omega = [0, 1]
u, c = least_squares(f, psi, Omega)
comparison_plot(f, u, Omega)
```

Figure 4 (left) shows the oscillatory approximation of $\sum_{j=0}^{N} c_j \sin((j+1)\pi x)$ when $N = 3$. Changing N to 11 improves the approximation considerably, see Figure 4 (right).

There is an error $f(0) - u(0) = 9$ at $x = 0$ in Figure 4 regardless of how large N is, because all $\psi_i(0) = 0$ and hence $u(0) = 0$. We may help the approximation to be correct at $x = 0$ by seeking

$$u(x) = f(0) + \sum_{j \in \mathcal{I}_s} c_j \psi_j(x). \tag{39}$$

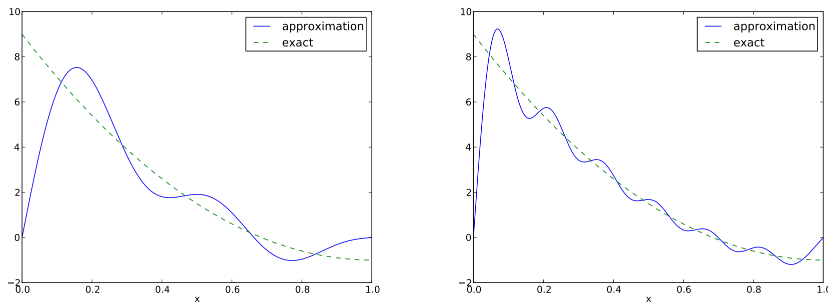


Figure 4: Best approximation of a parabola by a sum of 3 (left) and 11 (right) sine functions.

However, this adjustment introduces a new problem at $x = 1$ since we now get an error $f(1) - u(1) = f(1) - 0 = -1$ at this point. A more clever adjustment is to replace the $f(0)$ term by a term that is $f(0)$ at $x = 0$ and $f(1)$ at $x = 1$. A simple linear combination $f(0)(1 - x) + xf(1)$ does the job:

$$u(x) = f(0)(1 - x) + xf(1) + \sum_{j\in\mathcal{I}_s} c_j\psi_j(x)\,. \tag{40}$$

This adjustment of u alters the linear system slightly. In the general case, we set

$$u(x) = B(x) + \sum_{j\in\mathcal{I}_s} c_j\psi_j(x),$$

and the linear system becomes

$$\sum_{j\in\mathcal{I}_s} (\psi_i, \psi_j)c_j = (f - B, \psi_i), \quad i \in \mathcal{I}_s\,.$$

The calculations can still utilize the `least_squares` or `least_squares_orth` functions, but solve for $u - b$:

```
f0 = 0;  f1 = -1
B = f0*(1-x) + x*f1
u_sum, c = least_squares_orth(f-b, psi, Omega)
u = B + u_sum
```

Figure 5 shows the result of the technique for ensuring right boundary values. Even 3 sines can now adjust the $f(0)(1-x)+xf(1)$ term such that u approximates the parabola really well, at least visually.

2.8 Orthogonal basis functions

The choice of sine functions $\psi_i(x) = \sin((i + 1)\pi x)$ has a great computational advantage: on $\Omega = [0, 1]$ these basis functions are *orthogonal*, implying that $A_{i,j} = 0$ if $i \neq j$. This result is realized by trying

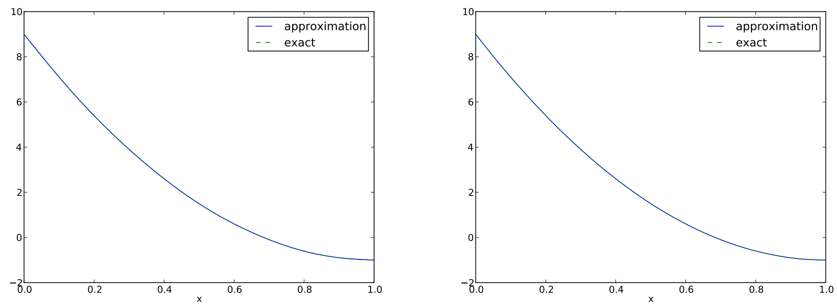


Figure 5: Best approximation of a parabola by a sum of 3 (left) and 11 (right) sine functions with a boundary term.

```
integrate(sin(j*pi*x)*sin(k*pi*x), x, 0, 1)
```

in WolframAlpha (avoid `i` in the integrand as this symbol means the imaginary unit $\sqrt{-1}$). Asking WolframAlpha also about $\int_0^1 \sin^2(j\pi x)\,\mathrm{d}x$, we find that it equals 1/2. With a diagonal matrix we can easily solve for the coefficients by hand:

$$c_i = 2\int_0^1 f(x)\sin((i+1)\pi x)\,\mathrm{d}x, \quad i\in\mathcal{I}_s, \tag{41}$$

which is nothing but the classical formula for the coefficients of the Fourier sine series of $f(x)$ on $[0,1]$. In fact, when V contains the basic functions used in a Fourier series expansion, the approximation method derived in Section 2 results in the classical Fourier series for $f(x)$ (see Exercise 8 for details).

With orthogonal basis functions we can make the `least_squares` function (much) more efficient since we know that the matrix is diagonal and only the diagonal elements need to be computed:

```
def least_squares_orth(f, psi, Omega):
    N = len(psi) - 1
    A = [0]*(N+1)
    b = [0]*(N+1)
    x = sym.Symbol('x')
    for i in range(N+1):
        A[i] = sym.integrate(psi[i]**2, (x, Omega[0], Omega[1]))
        b[i] = sym.integrate(psi[i]*f,  (x, Omega[0], Omega[1]))
    c = [b[i]/A[i] for i in range(len(b))]
    u = 0
    for i in range(len(psi)):
        u += c[i]*psi[i]
    return u, c
```

As mentioned in Section 2.4, symbolic integration may fail or take very long time. It is therefore natural to extend the implementation above with a version where we can choose between symbolic and numerical integration and fall back on the latter if the former fails:

```
def least_squares_orth(f, psi, Omega, symbolic=True):
    N = len(psi) - 1
    A = [0]*(N+1)       # plain list to hold symbolic expressions
    b = [0]*(N+1)
    x = sym.Symbol('x')
    for i in range(N+1):
        # Diagonal matrix term
        A[i] = sym.integrate(psi[i]**2, (x, Omega[0], Omega[1]))

        # Right-hand side term
        integrand = psi[i]*f
        if symbolic:
            I = sym.integrate(integrand,  (x, Omega[0], Omega[1]))
        if not symbolic or isinstance(I, sym.Integral):
            print 'numerical integration of', integrand
            integrand = sym.lambdify([x], integrand)
            I = sym.mpmath.quad(integrand, [Omega[0], Omega[1]])
        b[i] = I
    c = [b[i]/A[i] for i in range(len(b))]
    u = 0
    u = sum(c[i,0]*psi[i] for i in range(len(psi)))
    return u, c
```

This function is found in the file `approx1D.py`. Observe that we here assume that $\int_\Omega \varphi_i^2 \, dx$ can always be symbolically computed, which is not an unreasonable assumption when the basis functions are orthogonal, but there is no guarantee, so an improved version of the function above would implement numerical integration also for the `A[i,i]` term.

2.9 Numerical computations

Sometimes the basis functions ψ_i and/or the function f have a nature that makes symbolic integration CPU-time consuming or impossible. Even though we implemented a fall back on numerical integration of $\int f\varphi_i \, dx$, considerable time might still be required by `sympy` just by *attempting* to integrate symbolically. Therefore, it will be handy to have function for fast *numerical integration and numerical solution of the linear system.* Below is such a method. It requires Python functions `f(x)` and `psi(x,i)` for $f(x)$ and $\psi_i(x)$ as input. The output is a mesh function with values `u` on the mesh with points in the array `x`. Three numerical integration methods are offered: `scipy.integrate.quad` (precision set to 10^{-8}), `sympy.mpmath.quad` (about machine precision), and a Trapezoidal rule based on the points in `x` (unknown accuracy, but increasing with the number of mesh points in `x`).

```
def least_squares_numerical(f, psi, N, x,
                            integration_method='scipy',
                            orthogonal_basis=False):
    import scipy.integrate
    A = np.zeros((N+1, N+1))
    b = np.zeros(N+1)
    Omega = [x[0], x[-1]]
    dx = x[1] - x[0]

    for i in range(N+1):
        j_limit = i+1 if orthogonal_basis else N+1
```

```
        for j in range(i, j_limit):
            print '(%d,%d)' % (i, j)
            if integration_method == 'scipy':
                A_ij = scipy.integrate.quad(
                    lambda x: psi(x,i)*psi(x,j),
                    Omega[0], Omega[1], epsabs=1E-9, epsrel=1E-9)[0]
            elif integration_method == 'sympy':
                A_ij = sym.mpmath.quad(
                    lambda x: psi(x,i)*psi(x,j),
                    [Omega[0], Omega[1]])
            else:
                values = psi(x,i)*psi(x,j)
                A_ij = trapezoidal(values, dx)
            A[i,j] = A[j,i] = A_ij

        if integration_method == 'scipy':
            b_i = scipy.integrate.quad(
                lambda x: f(x)*psi(x,i), Omega[0], Omega[1],
                epsabs=1E-9, epsrel=1E-9)[0]
        elif integration_method == 'sympy':
            b_i = sym.mpmath.quad(
                lambda x: f(x)*psi(x,i), [Omega[0], Omega[1]])
        else:
            values = f(x)*psi(x,i)
            b_i = trapezoidal(values, dx)
        b[i] = b_i

    c = b/np.diag(A) if orthogonal_basis else np.linalg.solve(A, b)
    u = sum(c[i]*psi(x, i) for i in range(N+1))
    return u, c

def trapezoidal(values, dx):
    """Integrate values by the Trapezoidal rule (mesh size dx)."""
    return dx*(np.sum(values) - 0.5*values[0] - 0.5*values[-1])
```

Here is an example on calling the function:

```
from numpy import linspace, tanh, pi

def psi(x, i):
    return sin((i+1)*x)

x = linspace(0, 2*pi, 501)
N = 20
u, c = least_squares_numerical(lambda x: tanh(x-pi), psi, N, x,
                               orthogonal_basis=True)
```

2.10 The interpolation (or collocation) method

The principle of minimizing the distance between u and f is an intuitive way of computing a best approximation $u \in V$ to f. However, there are other approaches as well. One is to demand that $u(x_i) = f(x_i)$ at some selected points x_i, $i \in \mathcal{I}_s$:

$$u(x_i) = \sum_{j\in\mathcal{I}_s} c_j\psi_j(x_i) = f(x_i), \quad i \in \mathcal{I}_s\,. \tag{42}$$

We recognize that the equation $\sum_j c_j\psi_j(x_i) = f(x_i)$ is actually a linear system with $N+1$ unknown coefficients $\{c_j\}_{j\in\mathcal{I}_s}$:

$$\sum_{j\in\mathcal{I}_s} A_{i,j}c_j = b_i, \quad i\in\mathcal{I}_s, \tag{43}$$

with coefficient matrix and right-hand side vector given by

$$A_{i,j} = \psi_j(x_i), \tag{44}$$
$$b_i = f(x_i)\,. \tag{45}$$

This time the coefficient matrix is not symmetric because $\psi_j(x_i) \neq \psi_i(x_j)$ in general. The method is often referred to as an *interpolation method* since some point values of f are given ($f(x_i)$) and we fit a continuous function u that goes through the $f(x_i)$ points. In this case the x_i points are called *interpolation points*. When the same approach is used to approximate differential equations, one usually applies the name *collocation method* and x_i are known as *collocation points*.

Given f as a `sympy` symbolic expression `f`, $\{\psi_i\}_{i\in\mathcal{I}_s}$ as a list `psi`, and a set of points $\{x_i\}_{i\in\mathcal{I}_s}$ as a list or array `points`, the following Python function sets up and solves the matrix system for the coefficients $\{c_i\}_{i\in\mathcal{I}_s}$:

```
def interpolation(f, psi, points):
    N = len(psi) - 1
    A = sym.zeros((N+1, N+1))
    b = sym.zeros((N+1, 1))
    psi_sym = psi  # save symbolic expression
    # Turn psi and f into Python functions
    x = sym.Symbol('x')
    psi = [sym.lambdify([x], psi[i]) for i in range(N+1)]
    f = sym.lambdify([x], f)
    for i in range(N+1):
        for j in range(N+1):
            A[i,j] = psi[j](points[i])
        b[i,0] = f(points[i])
    c = A.LUsolve(b)
    # c is a sympy Matrix object, turn to list
    c = [sym.simplify(c[i,0]) for i in range(c.shape[0])]
    u = sym.simplify(sum(c[i,0]*psi_sym[i] for i in range(N+1)))
    return u, c
```

The `interpolation` function is a part of the `approx1D` module.

We found it convenient in the above function to turn the expressions `f` and `psi` into ordinary Python functions of `x`, which can be called with `float` values in the list `points` when building the matrix and the right-hand side. The alternative is to use the `subs` method to substitute the `x` variable in an expression by an element from the `points` list. The following session illustrates both approaches in a simple setting:

```
>>> import sympy as sym
>>> x = sym.Symbol('x')
>>> e = x**2              # symbolic expression involving x
>>> p = 0.5               # a value of x
>>> v = e.subs(x, p)      # evaluate e for x=p
>>> v
0.250000000000000
>>> type(v)
sympy.core.numbers.Float
>>> e = lambdify([x], e)  # make Python function of e
>>> type(e)
>>> function
>>> v = e(p)              # evaluate e(x) for x=p
>>> v
0.25
>>> type(v)
float
```

A nice feature of the interpolation or collocation method is that it avoids computing integrals. However, one has to decide on the location of the x_i points. A simple, yet common choice, is to distribute them uniformly throughout Ω.

Example. Let us illustrate the interpolation method by approximating our parabola $f(x) = 10(x-1)^2 - 1$ by a linear function on $\Omega = [1, 2]$, using two collocation points $x_0 = 1 + 1/3$ and $x_1 = 1 + 2/3$:

```
import sympy as sym
x = sym.Symbol('x')
f = 10*(x-1)**2 - 1
psi = [1, x]
Omega = [1, 2]
points = [1 + sym.Rational(1,3), 1 + sym.Rational(2,3)]
u, c = interpolation(f, psi, points)
comparison_plot(f, u, Omega)
```

The resulting linear system becomes

$$\left(\begin{array}{cc} 1 & 4/3 \\ 1 & 5/3 \end{array}\right)\left(\begin{array}{c} c_0 \\ c_1 \end{array}\right) = \left(\begin{array}{c} 1/9 \\ 31/9 \end{array}\right)$$

with solution $c_0 = -119/9$ and $c_1 = 10$. Figure 6 (left) shows the resulting approximation $u = -119/9 + 10x$. We can easily test other interpolation points, say $x_0 = 1$ and $x_1 = 2$. This changes the line quite significantly, see Figure 6 (right).

2.11 The regression method

The interpolation method in the previous section used exactly $N+1$ interpolation points. An alternative is to use $m+1 > N+1$ interpolation points $x_0, x_1, \ldots, x_m$. This is particularly relevant if f is just known through measured point values and we have many such values. The resulting method is called *regression* and is well known from statistics when fitting a simple (usually polynomial) function to a set of data points.

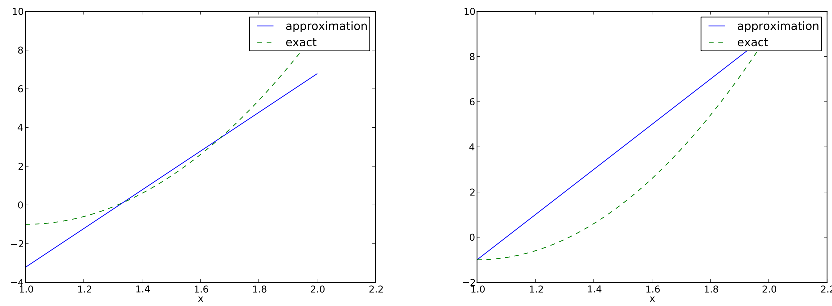


Figure 6: Approximation of a parabola by linear functions computed by two interpolation points: 4/3 and 5/3 (left) versus 1 and 2 (right).

Overdetermined equation system. Intuitively, we would demand u to equal f at all the data points x_i, $i0, 1, \ldots, m$,

$$u(x_i) = \sum_{j\in\mathcal{I}_s} c_j\psi_j(x_i) = f(x_i), \quad i = 0, 1, \ldots, m\,. \tag{46}$$

The fundamental problem here is that we have more equations than unknowns since there are $N+1$ unknowns and $m+1 > N+1$ equations. Such a system of equations is called an *overdetermined system*. We can write it matrix form as

$$\sum_{j\in\mathcal{I}_s} A_{i,j}c_j = b_i, \quad i = 0, 1, \ldots, m, \tag{47}$$

with coefficient matrix and right-hand side vector given by

$$A_{i,j} = \psi_j(x_i), \tag{48}$$
$$b_i = f(x_i)\,. \tag{49}$$

Note that the matrix is a *rectangular* $(m+1)\times(N+1)$ matrix since $i = 0, \ldots, m$ and $j = 0, \ldots, N$.

The normal equations derived from a least squares principle. The least squares method is a common technique for solving overdetermined equations systems. Let us write the overdetermined system $\sum_{j\in\mathcal{I}_s} A_{i,j}c_j = b_i$ more compactly in matrix form as $Ac = b$. Since we have more equations than unknowns, it is (in general) impossible to find a vector c that fulfills $Ac = b$. The best we can do is to make the residual $r = b - Ac$ as small as possible. That is, we can find c such it minimizes the norm Euclidean norm of r: $||r||$. The algebra simplifies significantly by minimizing $||r||^2$ instead. This principle corresponds to a least squares method.

The i-th component of r reads $r_i = b_i - \sum_j A_{i,j}c_j$, so $||r||^2 = \sum_i r_i^2$. Minimizing $||r||^2$ with respect to the unknowns $c_0, \ldots, c_N$ implies that

$$\frac{\partial}{\partial k}||r||^2 = 0, \quad k = 0, \ldots, N, \tag{50}$$

which leads to

$$\frac{\partial}{\partial k}\sum_i r_i^2 = \sum_i 2r_i\frac{\partial r_i}{\partial k} = \sum_i 2r_i\frac{\partial}{\partial k}(b_i - \sum_j A_{i,j}c_j) = 2\sum_i r_i(-A_{i,k}) = 0\,.$$

By inserting $r_i = b_i - \sum_j A_{i,j}c_j$ the last expression we get

$$\sum_i\left(b_i - \sum_j A_{i,j}c_j\right)(-A_{i,k}) = -\sum_i b_iA_{i,k} + \sum_j(\sum_i A_{i,j}A_{i,k})c_j = 0\,.$$

Introducing the transpose of A, A^T, we know that $A^T_{i,j} = A_{j,i}$, to the expression $\sum_i A_{i,j}A_{i,k}$ can be written as $\sum_i A^Tk, iA_{i,j}$ and recognized as the formula for the matrix-matrix product A^TA. Also, $\sum_i b_iA_{i,k}$ can be written $\sum_i A^T_{k,i}b_i$ and recognized as the matrix-vector product A^Tb. These observations imply that (50) is equivalent to the linear system

$$\sum_j(\underbrace{\sum_i A^Tk, iA_{i,j}} = (A^TA)_{k,j}c_j = \sum_i \underbrace{A^T_{k,i}b_i} = (A^Tb)_k, \quad k = 0, \ldots, N, \tag{51}$$

or in matrix form,

$$A^TA = A^Tb\,. \tag{52}$$

The equation system (51) or (52) are known as the *normal equations*. With A as an $(m+1)\times(N+1)$ matrix, A^TA becomes an $(N+1)\times(N+1)$ matrix, and A^Tb becomes a vector of length $N+1$. Often, $m \gg N$, so A^TA has much smaller size than A.

Many prefer to write the linear system (51) on the standard form $\sum_j B_{i,j} = d_i$, $i = 0, \ldots, N$. We can easily do so by exchanging the i and k index ($i \leftrightarrow k$), $\sum_i A^Tk, iA_{i,j} = \sum_k A^Ti, kA_{k,j}$, and setting $B_{i,j} = \sum_k A^Ti, kA_{k,j}$. Similarly, we exchange i and k in the right-hand side expression and get $\sum_k A^T_{i,k}b_k = d_i$. Expressing $B_{i,j}$ and d_i in terms of the ψ_i and x_i, using (48) and (49), we end up with the formulas

$$B_{i,j} = \sum_k A^Ti, kA_{k,j} = \sum_k Ak, iA_{k,j} = \sum_{k=0}^{m}\psi_i(x_k\psi_j(x_k, \tag{53}$$

$$d_i = \sum_k A^T_{i,k}b_k = \sum_k A_{k,i}b_k = \sum_{k=0}^{m}\psi_i(x_k)f(x_k) \tag{54}$$

Implementation. The following function defines the matrix entries $B_{i,j}$ according to (53) and the right-hand side entries d_i according (54). Thereafter, it solves the linear system $\sum_j B_{i,j}c_j = d_i$. The input data `f` and `psi` hold $f(x)$ and x_i, $i = 0, \ldots, N$, as symbolic expression, but since m is thought to be much larger than N, and there are loops from 0 to m, we use numerical computing to speed up the computations.

```
def regression(f, psi, points):
    N = len(psi) - 1
    m = len(points)
    # Use numpy arrays and numerical computing
    B = np.zeros((N+1, N+1))
    d = np.zeros(N+1)
    # Wrap psi and f in Python functions rather than expressions
    # so that we can evaluate psi at points[i]
    x = sym.Symbol('x')
    psi_sym = psi  # save symbolic expression
    psi = [sym.lambdify([x], psi[i]) for i in range(N+1)]
    f = sym.lambdify([x], f)
    for i in range(N+1):
        for j in range(N+1):
            B[i,j] = 0
            for k in range(m+1):
                B[i,j] += psi[i](points[k])*psi[j](points[k])
        d[i] = 0
        for k in range(m+1):
            d[i] += psi[i](points[k])*f(points[k])
    c = np.linalg.solve(B, d)
    u = sum(c[i]*psi_sym[i] for i in range(N+1))
    return u, c
```

Example. We repeat the computational example from Section 2.10, but this time with many more points. The parabola $f(x) = 10(x-1)^2 - 1$ is to be approximated by a linear function on $\Omega = [1, 2]$. We divide Ω into $m+2$ intervals and use the inner $m+1$ points:

```
import sympy as sym
x = sym.Symbol('x')
f = 10*(x-1)**2 - 1
psi = [1, x]
Omega = [1, 2]
m_values = [2-1, 8-1, 64-1]
# Create m+3 points and use the inner m+1 points
for m in m_values:
    points = np.linspace(Omega[0], Omega[1], m+3)[1:-1]
    u, c = regression(f, psi, points)
    comparison_plot(
        f, u, Omega,
        filename='parabola_by_regression_%d' % (m+1),
        points=points,
        points_legend='%d interpolation points' % (m+1),
        legend_loc='upper left')
```

Figure 7 shows results for $m+1 = 2$ (left), $m+1 = 8$ (middle), and $m+1 = 64$ (right) data points. The approximating function is not so sensitive to the number of points as long as they cover a significant part of the domain (2 points are too much in the middle, but 8 points cover almost the entire domain, and 64 points do not improve the results much):

$$
\begin{aligned}
u(x) &= 10x - 13.2, \quad \text{2 points}\\
u(x) &= 10x - 12.7, \quad \text{8 points}\\
u(x) &= 10x - 12.7, \quad \text{64 points}
\end{aligned}
$$

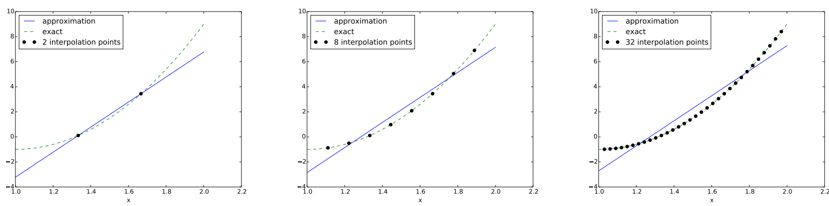


Figure 7: Approximation of a parabola by a regression method with varying number of points.

To explicitly make the link to classical regression in statistics, we consider $f = 10(x-1)^2 - 1 + \epsilon$, where ϵ is a random, normally distributed variable. The goal in classical regression is to find the straight line that best fits the data points (in a least squares sense). The only difference from the previous setup, is that the $f(x_i)$ values are based on a function formula, here $10(x-1)^2 - 1$, *plus* normally distributed noise. Figure 8 shows three sets of data points, along with the original $f(x)$ function without noise, and the straight line that is a least squares approximation to the data points.

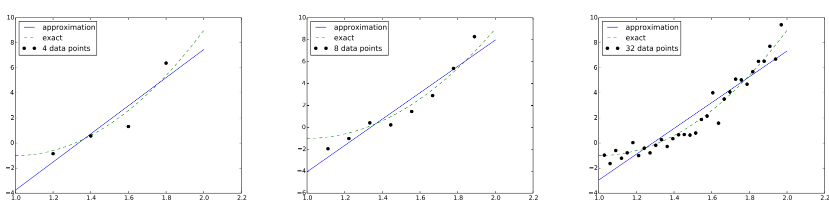


Figure 8: Approximation of a parabola with noise by a straight line.

We can fit a parabola instead of a straight line, as done in Figure 9. When m becomes large, the fitted parabola and the original parabola without noise become very close.

Remark. The regression method is not much used for approximating differential equations or given function, but is central in uncertainty quantification methods such as polynomial chaos expansions.

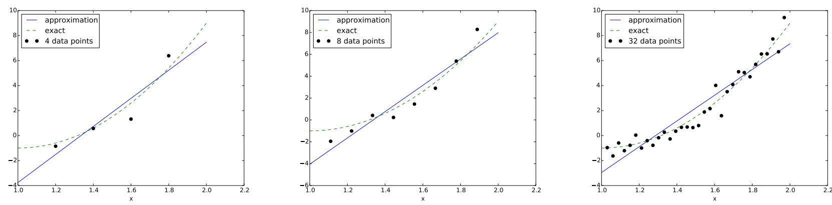


Figure 9: Approximation of a parabola with noise by a parabola.

2.12 Lagrange polynomials

In Section 2.7 we explained the advantage with having a diagonal matrix: formulas for the coefficients $\{c_i\}_{i\in\mathcal{I}_s}$ can then be derived by hand. For an interpolation (or collocation) method a diagonal matrix implies that $\psi_j(x_i) = 0$ if $i \neq j$. One set of basis functions $\psi_i(x)$ with this property is the *Lagrange interpolating polynomials*, or just *Lagrange polynomials*. (Although the functions are named after Lagrange, they were first discovered by Waring in 1779, rediscovered by Euler in 1783, and published by Lagrange in 1795.) Lagrange polynomials key building blocks in the finite element method, so familiarity with these polynomials will be required anyway.

A Lagrange polynomial can be written as

$$\psi_i(x) = \prod_{j=0,j\neq i}^{N} \frac{x - x_j}{x_i - x_j} = \frac{x - x_0}{x_i - x_0} \cdots \frac{x - x_{i-1}}{x_i - x_{i-1}} \frac{x - x_{i+1}}{x_i - x_{i+1}} \cdots \frac{x - x_N}{x_i - x_N}, \quad (55)$$

for $i \in \mathcal{I}_s$. We see from (55) that all the ψ_i functions are polynomials of degree N which have the property

$$\psi_i(x_s) = \delta_{is}, \quad \delta_{is} = \begin{cases} 1, & i = s, \\ 0, & i \neq s, \end{cases} \quad (56)$$

when x_s is an interpolation (collocation) point. Here we have used the *Kronecker delta* symbol δ_{is}. This property implies that $A_{i,j} = 0$ for $i \neq j$ and $A_{i,j} = 1$ when $i = j$. The solution of the linear system is then simply

$$c_i = f(x_i), \quad i \in \mathcal{I}_s, \quad (57)$$

and

$$u(x) = \sum_{j\in\mathcal{I}_s} f(x_i)\psi_i(x)\,. \quad (58)$$

The following function computes the Lagrange interpolating polynomial $\psi_i(x)$, given the interpolation points $x_0, \ldots, x_N$ in the list or array `points`:

```
def Lagrange_polynomial(x, i, points):
    p = 1
    for k in range(len(points)):
        if k != i:
            p *= (x - points[k])/(points[i] - points[k])
    return p
```

The next function computes a complete basis using equidistant points throughout Ω:

```
def Lagrange_polynomials_01(x, N):
    if isinstance(x, sym.Symbol):
        h = sym.Rational(1, N-1)
    else:
        h = 1.0/(N-1)
    points = [i*h for i in range(N)]
    psi = [Lagrange_polynomial(x, i, points) for i in range(N)]
    return psi, points
```

When `x` is an `sym.Symbol` object, we let the spacing between the interpolation points, `h`, be a `sympy` rational number, so that we get nice end results in the formulas for ψ_i. The other case, when `x` is a plain Python `float`, signifies numerical computing, and then we let `h` be a floating-point number. Observe that the `Lagrange_polynomial` function works equally well in the symbolic and numerical case - just think of `x` being an `sym.Symbol` object or a Python `float`. A little interactive session illustrates the difference between symbolic and numerical computing of the basis functions and points:

```
>>> import sympy as sym
>>> x = sym.Symbol('x')
>>> psi, points = Lagrange_polynomials_01(x, N=3)
>>> points
[0, 1/2, 1]
>>> psi
[(1 - x)*(1 - 2*x), 2*x*(2 - 2*x), -x*(1 - 2*x)]

>>> x = 0.5  # numerical computing
>>> psi, points = Lagrange_polynomials_01(x, N=3)
>>> points
[0.0, 0.5, 1.0]
>>> psi
[-0.0, 1.0, 0.0]
```

The Lagrange polynomials are very much used in finite element methods because of their property (56).

Approximation of a polynomial. The Galerkin or least squares method lead to an exact approximation if f lies in the space spanned by the basis functions. It could be of interest to see how the interpolation method with Lagrange polynomials as basis is able to approximate a polynomial, e.g., a parabola. Running

```
for N in 2, 4, 5, 6, 8, 10, 12:
    f = x**2
    psi, points = Lagrange_polynomials_01(x, N)
    u = interpolation(f, psi, points)
```

shows the result that up to `N=4` we achieve an exact approximation, and then round-off errors start to grow, such that `N=15` leads to a 15-degree polynomial for u where the coefficients in front of x^r for $r > 2$ are of size 10^{-5} and smaller.

Successful example. Trying out the Lagrange polynomial basis for approximating $f(x) = \sin 2\pi x$ on $\Omega = [0, 1]$ with the least squares and the interpolation techniques can be done by

```
x = sym.Symbol('x')
f = sym.sin(2*sym.pi*x)
psi, points = Lagrange_polynomials_01(x, N)
Omega=[0, 1]
u, c = least_squares(f, psi, Omega)
comparison_plot(f, u, Omega)
u, c = interpolation(f, psi, points)
comparison_plot(f, u, Omega)
```

Figure 10 shows the results. There is little difference between the least squares and the interpolation technique. Increasing N gives visually better approximations.

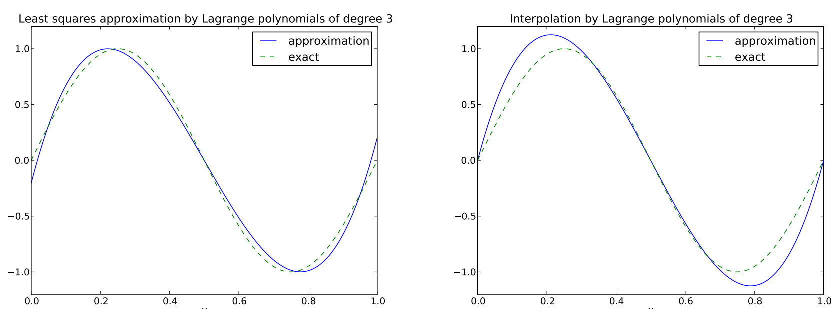


Figure 10: Approximation via least squares (left) and interpolation (right) of a sine function by Lagrange interpolating polynomials of degree 3.

Less successful example. The next example concerns interpolating $f(x) = |1 - 2x|$ on $\Omega = [0, 1]$ using Lagrange polynomials. Figure 11 shows a peculiar effect: the approximation starts to oscillate more and more as N grows. This numerical artifact is not surprising when looking at the individual Lagrange polynomials. Figure 12 shows two such polynomials, $\psi_2(x)$ and $\psi_7(x)$, both of degree 11 and computed from uniformly spaced points $x_{x_i} = i/11$, $i = 0, \ldots, 11$, marked with circles. We clearly see the property of Lagrange polynomials: $\psi_2(x_i) = 0$ and $\psi_7(x_i) = 0$ for all i, except $\psi_2(x_2) = 1$ and $\psi_7(x_7) = 1$. The most striking feature, however, is the significant oscillation near the boundary.

The reason is easy to understand: since we force the functions to zero at so many points, a polynomial of high degree is forced to oscillate between the points. The phenomenon is named *Runge's phenomenon* and you can read a more detailed explanation on Wikipedia.

Remedy for strong oscillations. The oscillations can be reduced by a more clever choice of interpolation points, called the *Chebyshev nodes*:

$$x_i = \frac{1}{2}(a+b) + \frac{1}{2}(b-a)\cos\left(\frac{2i+1}{2(N+1)}pi\right), \quad i = 0\ldots, N, \tag{59}$$

on the interval $\Omega = [a,b]$. Here is a flexible version of the `Lagrange_polynomials_01` function above, valid for any interval $\Omega = [a,b]$ and with the possibility to generate both uniformly distributed points and Chebyshev nodes:

```
def Lagrange_polynomials(x, N, Omega, point_distribution='uniform'):
    if point_distribution == 'uniform':
        if isinstance(x, sym.Symbol):
            h = sym.Rational(Omega[1] - Omega[0], N)
        else:
            h = (Omega[1] - Omega[0])/float(N)
        points = [Omega[0] + i*h for i in range(N+1)]
    elif point_distribution == 'Chebyshev':
        points = Chebyshev_nodes(Omega[0], Omega[1], N)
    psi = [Lagrange_polynomial(x, i, points) for i in range(N+1)]
    return psi, points

def Chebyshev_nodes(a, b, N):
    from math import cos, pi
    return [0.5*(a+b) + 0.5*(b-a)*cos(float(2*i+1)/(2*N+1))*pi) \
            for i in range(N+1)]
```

All the functions computing Lagrange polynomials listed above are found in the module file `Lagrange.py`.

Figure 13 shows the improvement of using Chebyshev nodes, compared with the equidistant points in Figure 11. The reason for this improvement is that the corresponding Lagrange polynomials have much smaller oscillations, which can be seen by comparing Figure 14 (Chebyshev points) with Figure 12 (equidistant points). Note the different scale on the vertical axes in the two figures.

Another cure for undesired oscillations of higher-degree interpolating polynomials is to use lower-degree Lagrange polynomials on many small patches of the domain. This is actually the idea pursued in the finite element method. For instance, linear Lagrange polynomials on $[0,1/2]$ and $[1/2,1]$ would yield a perfect approximation to $f(x) = |1-2x|$ on $\Omega = [0,1]$ since f is piecewise linear.

How does the least squares or projection methods work with Lagrange polynomials? We can just call the `least_squares` function, but `sympy` has problems integrating the $f(x) = |1-2x|$ function times a polynomial, so we need to fall back on numerical integration.

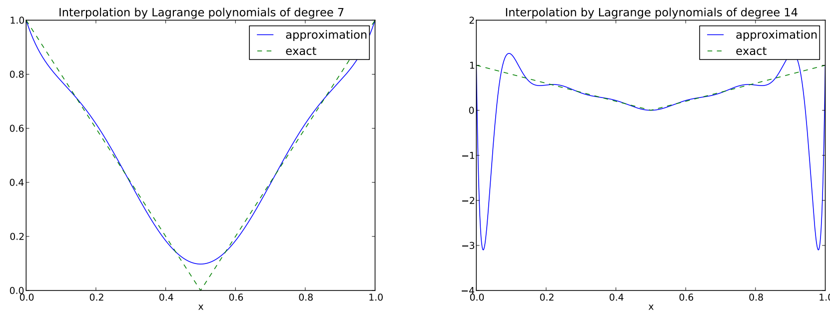


Figure 11: Interpolation of an absolute value function by Lagrange polynomials and uniformly distributed interpolation points: degree 7 (left) and 14 (right).

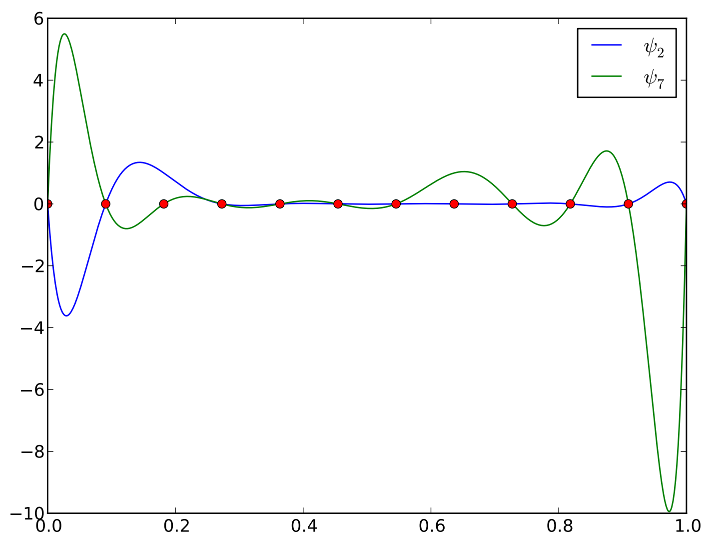


Figure 12: Illustration of the oscillatory behavior of two Lagrange polynomials based on 12 uniformly spaced points (marked by circles).

```
def least_squares(f, psi, Omega):
    N = len(psi) - 1
    A = sym.zeros((N+1, N+1))
    b = sym.zeros((N+1, 1))
    x = sym.Symbol('x')
    for i in range(N+1):
        for j in range(i, N+1):
            integrand = psi[i]*psi[j]
            I = sym.integrate(integrand, (x, Omega[0], Omega[1]))
            if isinstance(I, sym.Integral):
```

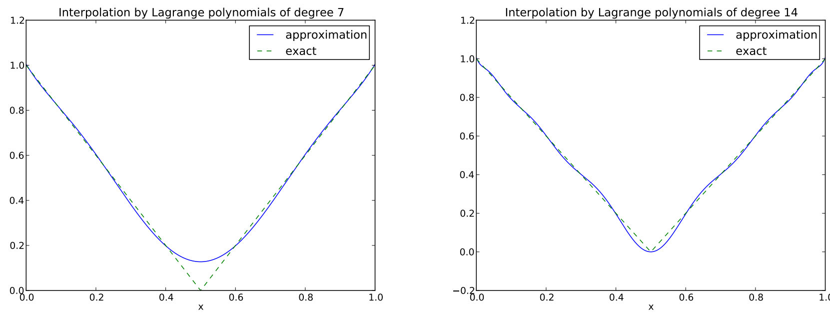


Figure 13: Interpolation of an absolute value function by Lagrange polynomials and Chebyshev nodes as interpolation points: degree 7 (left) and 14 (right).

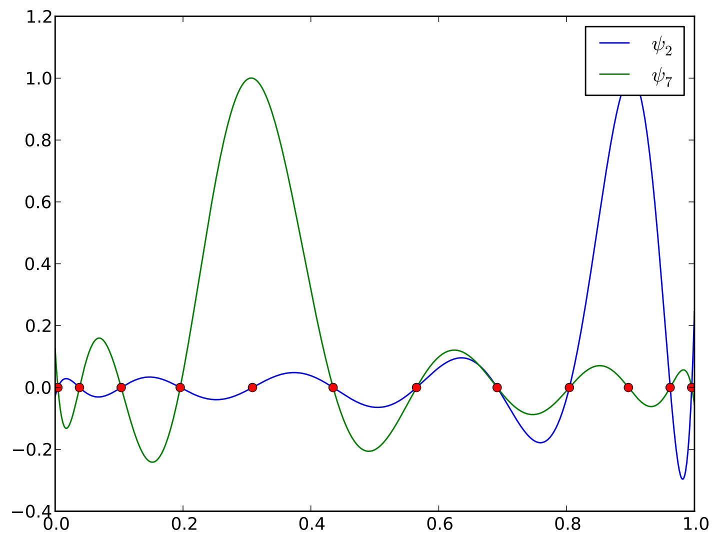


Figure 14: Illustration of the less oscillatory behavior of two Lagrange polynomials based on 12 Chebyshev points (marked by circles).

```
                # Could not integrate symbolically, fall back
                # on numerical integration with mpmath.quad
                integrand = sym.lambdify([x], integrand)
                I = sym.mpmath.quad(integrand, [Omega[0], Omega[1]])
            A[i,j] = A[j,i] = I
        integrand = psi[i]*f
        I = sym.integrate(integrand, (x, Omega[0], Omega[1]))
        if isinstance(I, sym.Integral):
            integrand = sym.lambdify([x], integrand)
            I = sym.mpmath.quad(integrand, [Omega[0], Omega[1]])
        b[i,0] = I
```

```
    c = A.LUsolve(b)
    c = [sym.simplify(c[i,0]) for i in range(c.shape[0])]
    u = sum(c[i]*psi[i] for i in range(len(psi)))
    return u, c
```

The idea of avoiding oscillatory solutions by using lower-order Lagrange polynomials on smaller patches throughout the domain, is important in the finite element method, and the next section introduces finite element basis functions based on Lagrange polynomials.

3 Finite element basis functions

The specific basis functions exemplified in Section 2 are in general nonzero on the entire domain Ω, as can be seen in Figure 15, where we plot two sinusoidal basis functions $\psi_0(x) = \sin \frac{1}{2}\pi x$ and $\psi_1(x) = \sin 2\pi x$ together with the sum $u(x) = 4\psi_0(x) - \frac{1}{2}\psi_1(x)$. We shall now turn our attention to basis functions that have *compact support*, meaning that they are nonzero on a small portion of Ω only. Moreover, we shall restrict the functions to be *piecewise polynomials*. This means that the domain is split into subdomains and each basis function is a polynomial on one or more of these subdomains, see Figure 16 for a sketch involving locally defined hat functions that make $u = \sum_j c_j\psi_j$ piecewise linear. At the boundaries between subdomains, one normally just forces continuity of u, so that when connecting two polynomials from two subdomains, the derivative becomes discontinuous. This type of basis functions is fundamental in the finite element method. (One may wonder why continuity of derivatives is not desired, and it is, but it turns out to be mathematically challenging in 2D and 3D, and it is not strictly needed.)

We first introduce the concepts of elements and nodes in a simplistic fashion, as often met in the literature. Later, we shall generalize the concept of an element, which is a necessary step before treating a wider class of approximations within the family of finite element methods. The generalization is also compatible with the concepts used in the FEniCS finite element software.

3.1 Elements and nodes

Let u and f be defined on an interval Ω. We divide Ω into N_e non-overlapping subintervals $\Omega^{(e)}$, $e = 0, \ldots, N_e - 1$:

$$\Omega = \Omega^{(0)} \cup \cdots \cup \Omega^{(N_e)}\,. \tag{60}$$

We shall for now refer to $\Omega^{(e)}$ as an *element*, identified by the unique number e. On each element we introduce a set of points called *nodes*. For now we assume that the nodes are uniformly spaced throughout the element and that the boundary points of the elements are also nodes. The nodes are given numbers both within an element and in the global domain. These are referred to as *local* and *global* node numbers, respectively. Local nodes are numbered with an index $r = 0, \ldots, d$, while the N_n global nodes are numbered as $i = 0, \ldots, N_n - 1$.

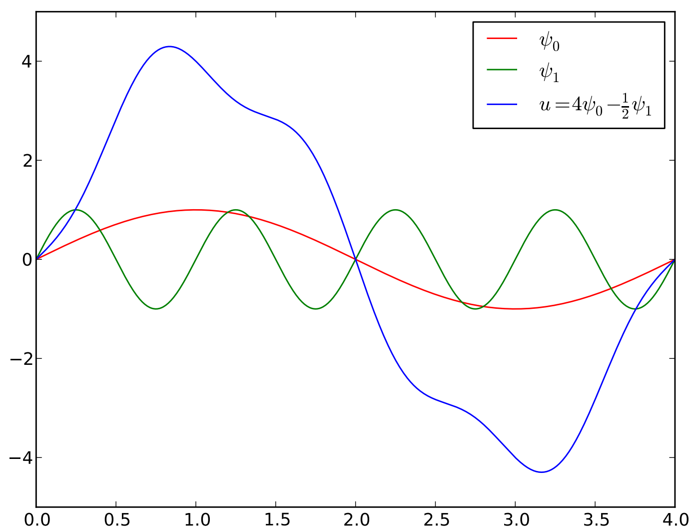


Figure 15: A function resulting from a weighted sum of two sine basis functions.

Figure 17 shows nodes as small circular disks and element boundaries as small vertical lines. Global node numbers appear under the nodes, but local node numbers are not shown. Since there are two nodes in each elements, the local nodes are numbered 0 (left) and 1 (right) in each element.

Nodes and elements uniquely define a *finite element mesh*, which is our discrete representation of the domain in the computations. A common special case is that of a *uniformly partitioned mesh* where each element has the same length and the distance between nodes is constant. Figure 17 shows an example on a uniformly partitioned mesh. The strength of the finite element method (in contrast to the finite difference method) is that it is equally easy to work with a non-uniformly partitioned mesh as a uniformly partitioned one.

Example. On $\Omega = [0,1]$ we may introduce two elements, $\Omega^{(0)} = [0, 0.4]$ and $\Omega^{(1)} = [0.4, 1]$. Furthermore, let us introduce three nodes per element, equally spaced within each element. Figure 18 shows the mesh with $N_e = 2$ elements and $N_n = 2N_e + 1 = 5$ nodes. A node's coordinate is denoted by x_i, where i is either a global node number or a local one. In the latter case we also need to know the element number to uniquely define the node.

The three nodes in element number 0 are $x_0 = 0$, $x_1 = 0.2$, and $x_2 = 0.4$. The local and global node numbers are here equal. In element number 1, we have the local nodes $x_0 = 0.4$, $x_1 = 0.7$, and $x_2 = 1$ and the corresponding

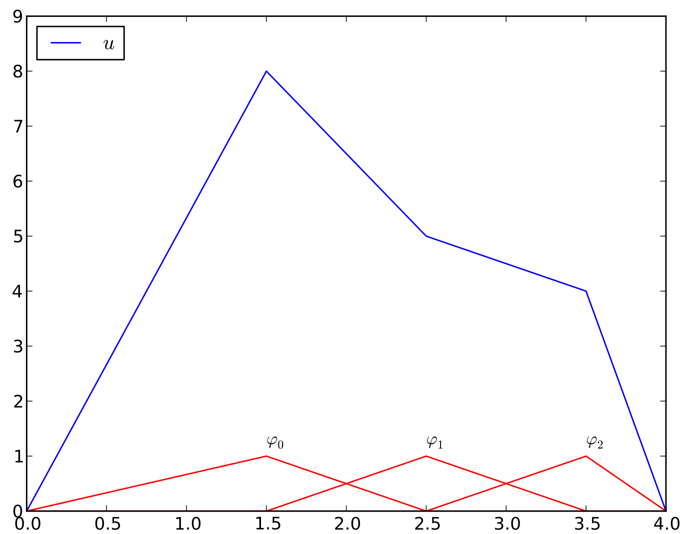


Figure 16: A function resulting from a weighted sum of three local piecewise linear (hat) functions.

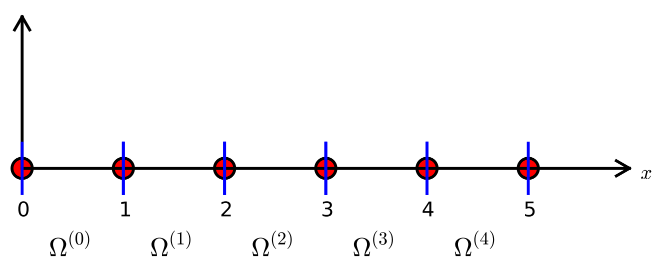


Figure 17: Finite element mesh with 5 elements and 6 nodes.

global nodes $x_2 = 0.4$, $x_3 = 0.7$, and $x_4 = 1$. Note that the global node $x_2 = 0.4$ is shared by the two elements.

For the purpose of implementation, we introduce two lists or arrays: `nodes` for storing the coordinates of the nodes, with the global node numbers as indices, and `elements` for holding the global node numbers in each element. By defining `elements` as a list of lists, where each sublist contains the global node numbers of one particular element, the indices of each sublist will correspond to local node numbers for that element. The `nodes` and `elements` lists for the sample mesh above take the form

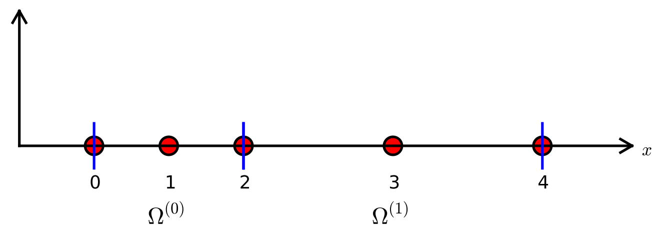


Figure 18: Finite element mesh with 2 elements and 5 nodes.

```
nodes = [0, 0.2, 0.4, 0.7, 1]
elements = [[0, 1, 2], [2, 3, 4]]
```

Looking up the coordinate of, e.g., local node number 2 in element 1, is done by `nodes[elements[1][2]]` (recall that nodes and elements start their numbering at 0). The corresponding global node number is 4, so we could alternatively look up the coordinate as `nodes[4]`.

The numbering of elements and nodes does not need to be regular. Figure 19 shows and example corresponding to

```
nodes = [1.5, 5.5, 4.2, 0.3, 2.2, 3.1]
elements = [[2, 1], [4, 5], [0, 4], [3, 0], [5, 2]]
```

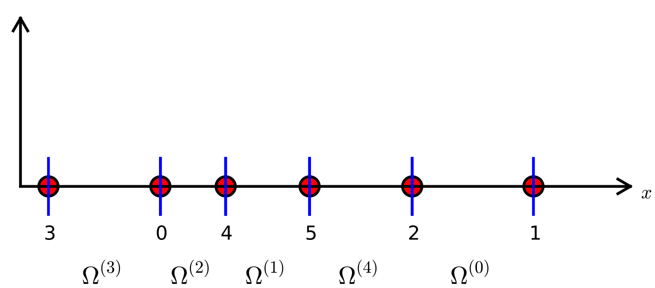


Figure 19: Example on irregular numbering of elements and nodes.

3.2 The basis functions

Construction principles. Finite element basis functions are in this text recognized by the notation $\varphi_i(x)$, where the index (now in the beginning) corresponds to a global node number. Since φ_i is the symbol for basis functions in general in this text, the particular choice of finite element basis functions means that we take $\psi_i = \varphi_i$.

Let i be the global node number corresponding to local node r in element number e with $d+1$ local nodes. We distinguish between *internal* nodes in an element and *shared* nodes. The latter are nodes that are shared with the neighboring elements. The finite element basis functions φ_i are now defined as follows.

- For an internal node, with global number i and local number r, take $\varphi_i(x)$ to be the Lagrange polynomial that is 1 at the local node r and zero at all other nodes in the element. The degree of the polynomial is d, according to (55). On all other elements, $\varphi_i = 0$.
- For a shared node, let φ_i be made up of the Lagrange polynomial on this element that is 1 at node i, combined with the Lagrange polynomial over the neighboring element that is also 1 at node i. On all other elements, $\varphi_i = 0$.

A visual impression of three such basis functions is given in Figure 20. The domain $\Omega = [0, 1]$ is divided into four equal-sized elements, each having three local nodes. The element boundaries are marked by vertical dashed lines and the nodes by small circles. The function $\varphi_2(x)$ is composed of a quadratic Lagrange polynomial over element 0 and 1, $\varphi_3(x)$ corresponds to an internal node in element 1 and is therefore nonzero on this element only, while $\varphi_4(x)$ is like $\varphi_2(x)$ composed to two Lagrange polynomials over two elements. Also observe that the basis function φ_i is zero at all nodes, except at global node number i. We also remark that the shape of a basis function over an element is completely determined by the coordinates of the local nodes in the element.

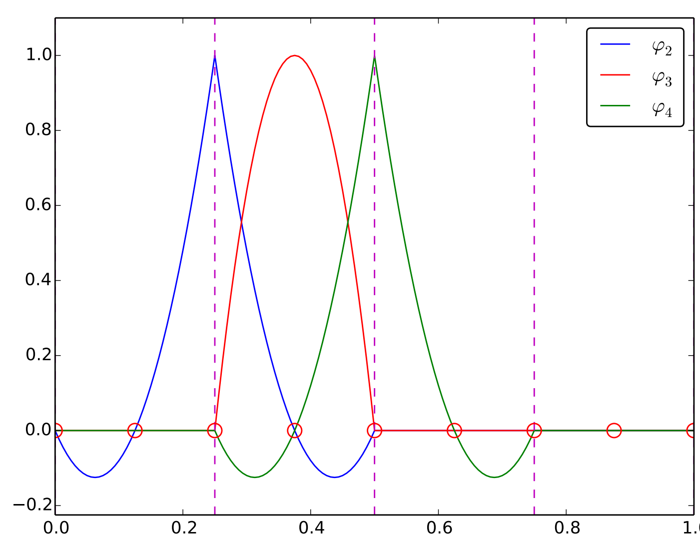


Figure 20: Illustration of the piecewise quadratic basis functions associated with nodes in an element.

Properties of φ_i. The construction of basis functions according to the principles above lead to two important properties of $\varphi_i(x)$. First,

$$\varphi_i(x_j) = \delta_{ij}, \quad \delta_{ij} = \begin{cases} 1, & i = j, \\ 0, & i \neq j, \end{cases} \tag{61}$$

when x_j is a node in the mesh with global node number j. The result $\varphi_i(x_j) = \delta_{ij}$ arises because the Lagrange polynomials are constructed to have exactly this property. The property also implies a convenient interpretation of c_i as the value of u at node i. To show this, we expand u in the usual way as $\sum_j c_j\psi_j$ and choose $\psi_i = \varphi_i$:

$$u(x_i) = \sum_{j\in\mathcal{I}_s} c_j\psi_j(x_i) = \sum_{j\in\mathcal{I}_s} c_j\varphi_j(x_i) = c_i\varphi_i(x_i) = c_i\,.$$

Because of this interpretation, the coefficient c_i is by many named u_i or U_i.

Second, $\varphi_i(x)$ is mostly zero throughout the domain:

- $\varphi_i(x) \neq 0$ only on those elements that contain global node i,
- $\varphi_i(x)\varphi_j(x) \neq 0$ if and only if i and j are global node numbers in the same element.

Since $A_{i,j}$ is the integral of $\varphi_i\varphi_j$ it means that *most of the elements in the coefficient matrix will be zero*. We will come back to these properties and use them actively in computations to save memory and CPU time.

In our example so far, each element has $d + 1$ nodes, resulting in local Lagrange polynomials of degree d (according to Section 2.12), but it is not a requirement to have the same d value in each element.

3.3 Example on piecewise quadratic finite element functions

Let us set up the `nodes` and `elements` lists corresponding to the mesh implied by Figure 20. Figure 21 sketches the mesh and the numbering. We have

```
nodes = [0, 0.125, 0.25, 0.375, 0.5, 0.625, 0.75, 0.875, 1.0]
elements = [[0, 1, 2], [2, 3, 4], [4, 5, 6], [6, 7, 8]]
```

Let us explain in mathematically how the basis functions are constructed according to the principles. Consider element number 1 in Figure 21, $\Omega^{(1)} = [0.25, 0.5]$, with local nodes 0, 1, and 2 corresponding to global nodes 2, 3, and 4. The coordinates of these nodes are 0.25, 0.375, and 0.5, respectively. We define three Lagrange polynomials on this element:

1. The polynomial that is 1 at local node 1 (global node 3) makes up the basis function $\varphi_3(x)$ over this element, with $\varphi_3(x) = 0$ outside the element.

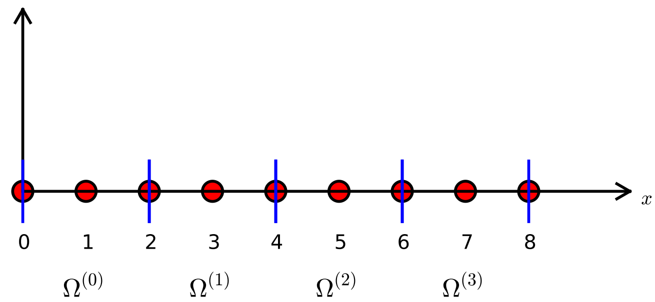


Figure 21: Sketch of mesh with 4 elements and 3 nodes per element.

2. The polynomial that is 1 at local node 0 (global node 2) is the "right part" of the global basis function $\varphi_2(x)$. The "left part" of $\varphi_2(x)$ consists of a Lagrange polynomial associated with local node 2 in the neighboring element $\Omega^{(0)} = [0, 0.25]$.

3. Finally, the polynomial that is 1 at local node 2 (global node 4) is the "left part" of the global basis function $\varphi_4(x)$. The "right part" comes from the Lagrange polynomial that is 1 at local node 0 in the neighboring element $\Omega^{(2)} = [0.5, 0.75]$.

The specific mathematical form of the polynomials *over element* 1 is given by the formula (55):

$$\varphi_3(x) = \frac{(x-0.25)(x-0.5)}{(0.375-0.25)(0.375-0.5)}, \quad x \in \Omega^{(1)}$$
$$\varphi_2(x) = \frac{(x-0.375)(x-0.5)}{(0.25-0.375)(0.25-0.5)}, \quad x \in \Omega^{(1)}$$
$$\varphi_4(x) = \frac{(x-0.25)(x-0.375)}{(0.5-0.25)(0.5-0.25)}, \quad x \in \Omega^{(1)}$$

As mentioned earlier, any global basis function $\varphi_i(x)$ is zero on elements that do not contain the node with global node number i.

The other global functions associated with internal nodes, φ_1, φ_5, and φ_7, are all of the same shape as the drawn φ_3 in Figure 20, while the global basis functions associated with shared nodes have the same shape as shown φ_2 and φ_4. If the elements were of different length, the basis functions would be stretched according to the element size and hence be different.

3.4 Example on piecewise linear finite element functions

Figure 22 shows piecewise linear basis functions ($d = 1$). These are mathematically simpler than the quadratic functions in the previous section, and one would therefore think that it is easier to understand the linear functions first. However, linear basis functions do not involve internal nodes and are therefore a special case of the general situation. That is why we think it is better to understand the construction of quadratic functions first, which easily generalize to any $d > 2$, and then look at the special case $d = 1$.

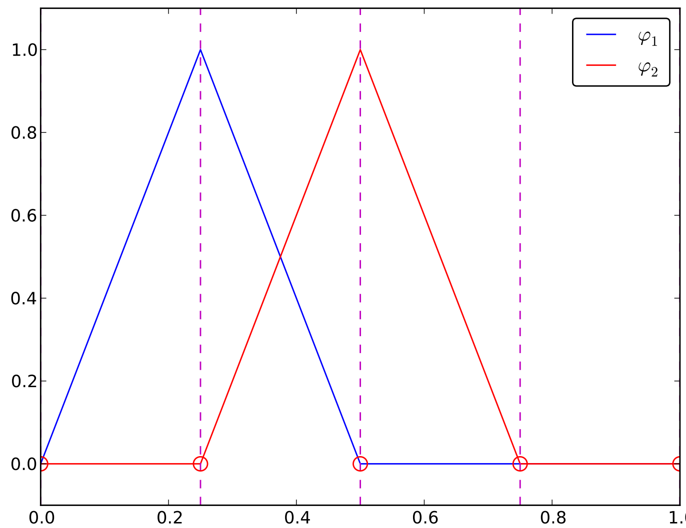


Figure 22: Illustration of the piecewise linear basis functions associated with nodes in an element.

We have the same four elements on $\Omega = [0, 1]$. Now there are no internal nodes in the elements so that all basis functions are associated with shared nodes and hence made up of two Lagrange polynomials, one from each of the two neighboring elements. For example, $\varphi_1(x)$ results from the Lagrange polynomial in element 0 that is 1 at local node 1 and 0 at local node 0, combined with the Lagrange polynomial in element 1 that is 1 at local node 0 and 0 at local node 1. The other basis functions are constructed similarly.

Explicit mathematical formulas are needed for $\varphi_i(x)$ in computations. In the piecewise linear case, the formula (55) leads to

$$\varphi_i(x) = \begin{cases} 0, & x < x_{i-1}, \\ (x - x_{i-1})/(x_i - x_{i-1}), & x_{i-1} \le x < x_i, \\ 1 - (x - x_i)/(x_{i+1} - x_i), & x_i \le x < x_{i+1}, \\ 0, & x \ge x_{i+1}\,. \end{cases} \tag{62}$$

Here, x_j, $j = i-1, i, i+1$, denotes the coordinate of node j. For elements of equal length h the formulas can be simplified to

$$\varphi_i(x) = \begin{cases} 0, & x < x_{i-1}, \\ (x - x_{i-1})/h, & x_{i-1} \leq x < x_i, \\ 1 - (x - x_i)/h, & x_i \leq x < x_{i+1}, \\ 0, & x \geq x_{i+1} \end{cases} \tag{63}$$

3.5 Example on piecewise cubic finite element basis functions

Piecewise cubic basis functions can be defined by introducing four nodes per element. Figure 23 shows examples on $\varphi_i(x)$, $i = 3, 4, 5, 6$, associated with element number 1. Note that φ_4 and φ_5 are nonzero on element number 1, while φ_3 and φ_6 are made up of Lagrange polynomials on two neighboring elements.

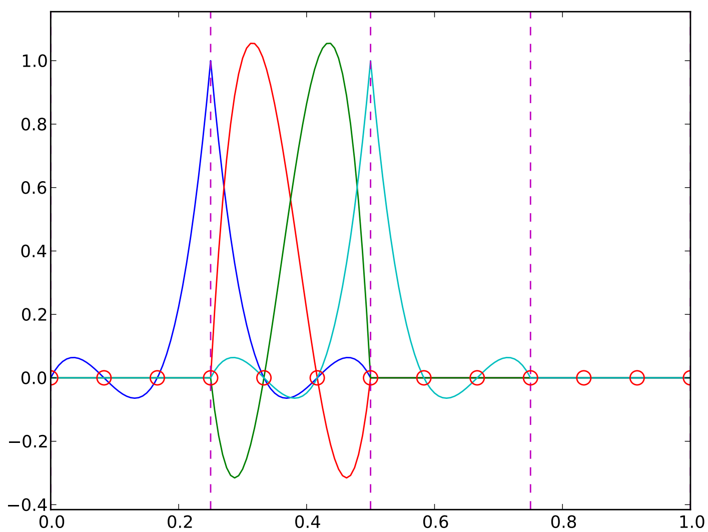


Figure 23: Illustration of the piecewise cubic basis functions associated with nodes in an element.

We see that all the piecewise linear basis functions have the same "hat" shape. They are naturally referred to as *hat functions*, also called *chapeau functions*. The piecewise quadratic functions in Figure 20 are seen to be of two types. "Rounded hats" associated with internal nodes in the elements and some more "sombrero" shaped hats associated with element boundary nodes. Higher-order basis functions also have hat-like shapes, but the functions have pronounced oscillations in addition, as illustrated in Figure 23.

A common terminology is to speak about *linear elements* as elements with two local nodes associated with piecewise linear basis functions. Similarly, *quadratic* *elements* and *cubic elements* refer to piecewise quadratic or cubic functions over elements with three or four local nodes, respectively. Alternative names, frequently used in the following, are P1 elements for linear elements, P2 for quadratic elements, and so forth: Pd signifies degree d of the polynomial basis functions.

3.6 Calculating the linear system

The elements in the coefficient matrix and right-hand side are given by the formulas (27) and (28), but now the choice of ψ_i is φ_i. Consider P1 elements where $\varphi_i(x)$ is piecewise linear. Nodes and elements numbered consecutively from left to right in a uniformly partitioned mesh imply the nodes

$$x_i = ih, \quad i = 0, \ldots, N_n - 1,$$

and the elements

$$\Omega^{(i)} = [x_i, x_{i+1}] = [ih, (i+1)h], \quad i = 0, \ldots, N_e - 1\,. \tag{64}$$

We have in this case N_e elements and $N_n = N_e + 1$ nodes. The parameter N denotes the number of unknowns in the expansion for u, and with the P1 elements, $N = N_n - 1$. The domain is $\Omega = [x_0, x_N]$. The formula for $\varphi_i(x)$ is given by (63) and a graphical illustration is provided in Figures 22 and 25.

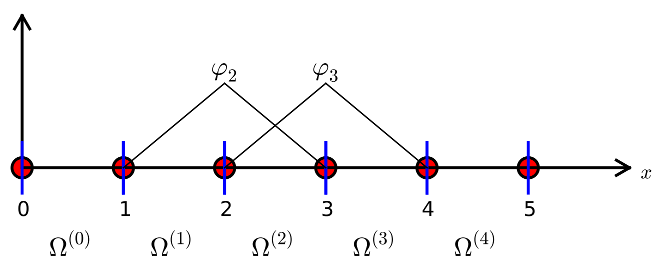


Figure 24: Illustration of the piecewise linear basis functions corresponding to global node 2 and 3.

Calculating specific matrix entries. Let us calculate the specific matrix entry $A_{2,3} = \int_\Omega \varphi_2\varphi_3 \,\mathrm{d}x$. Figure 24 shows what φ_2 and φ_3 look like. We realize from this figure that the product $\varphi_2\varphi_3 \neq 0$ only over element 2, which contains node 2 and 3. The particular formulas for $\varphi_2(x)$ and $\varphi_3(x)$ on $[x_2, x_3]$ are found from (63). The function φ_3 has positive slope over $[x_2, x_3]$ and corresponds to the interval $[x_{i-1}, x_i]$ in (63). With $i = 3$ we get

$$\varphi_3(x) = (x - x_2)/h,$$

while $\varphi_2(x)$ has negative slope over $[x_2, x_3]$ and corresponds to setting $i = 2$ in (63),

$$\varphi_2(x) = 1 - (x - x_2)/h\,.$$

We can now easily integrate,

$$A_{2,3} = \int_\Omega \varphi_2\varphi_3\,\mathrm{d}x = \int_{x_2}^{x_3}\left(1 - \frac{x - x_2}{h}\right)\frac{x - x_2}{h}\,\mathrm{d}x = \frac{h}{6}\,.$$

The diagonal entry in the coefficient matrix becomes

$$A_{2,2} = \int_{x_1}^{x_2}\left(\frac{x - x_1}{h}\right)^2 \mathrm{d}x + \int_{x_2}^{x_3}\left(1 - \frac{x - x_2}{h}\right)^2 \mathrm{d}x = \frac{2h}{3}\,.$$

The entry $A_{2,1}$ has an integral that is geometrically similar to the situation in Figure 24, so we get $A_{2,1} = h/6$.

Calculating a general row in the matrix. We can now generalize the calculation of matrix entries to a general row number i. The entry $A_{i,i-1} = \int_\Omega \varphi_i\varphi_{i-1}\,\mathrm{d}x$ involves hat functions as depicted in Figure 25. Since the integral is geometrically identical to the situation with specific nodes 2 and 3, we realize that $A_{i,i-1} = A_{i,i+1} = h/6$ and $A_{i,i} = 2h/3$. However, we can compute the integral directly too:

$$\begin{aligned}
A_{i,i-1} &= \int_\Omega \varphi_i\varphi_{i-1}\,\mathrm{d}x\\
&= \underbrace{\int_{x_{i-2}}^{x_{i-1}} \varphi_i\varphi_{i-1}\,\mathrm{d}x}_{\varphi_i=0} + \int_{x_{i-1}}^{x_i} \varphi_i\varphi_{i-1}\,\mathrm{d}x + \underbrace{\int_{x_i}^{x_{i+1}} \varphi_i\varphi_{i-1}\,\mathrm{d}x}_{\varphi_{i-1}=0}\\
&= \int_{x_{i-1}}^{x_i} \underbrace{\left(\frac{x - x_i}{h}\right)}_{\varphi_i(x)}\underbrace{\left(1 - \frac{x - x_{i-1}}{h}\right)}_{\varphi_{i-1}(x)}\mathrm{d}x = \frac{h}{6}\,.
\end{aligned}$$

The particular formulas for $\varphi_{i-1}(x)$ and $\varphi_i(x)$ on $[x_{i-1}, x_i]$ are found from (63): φ_i is the linear function with positive slope, corresponding to the interval $[x_{i-1}, x_i]$ in (63), while ϕ_{i-1} has a negative slope so the definition in interval $[x_i, x_{i+1}]$ in (63) must be used.

The first and last row of the coefficient matrix lead to slightly different integrals:

$$A_{0,0} = \int_\Omega \varphi_0^2\,\mathrm{d}x = \int_{x_0}^{x_1}\left(1 - \frac{x - x_0}{h}\right)^2 \mathrm{d}x = \frac{h}{3}\,.$$

Similarly, $A_{N,N}$ involves an integral over only one element and hence equals $h/3$.

The general formula for b_i, see Figure 26, is now easy to set up

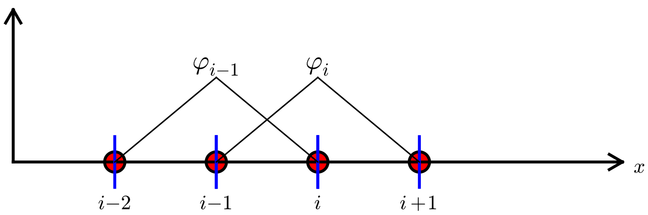


Figure 25: Illustration of two neighboring linear (hat) functions with general node numbers.

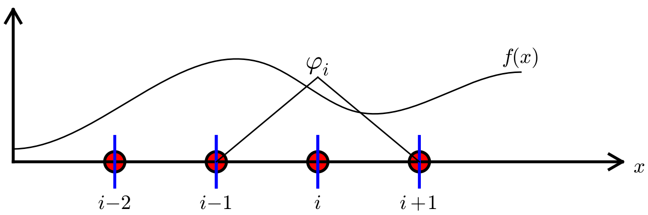


Figure 26: Right-hand side integral with the product of a basis function and the given function to approximate.

$$b_i = \int_\Omega \varphi_i(x) f(x)\,\mathrm{d}x = \int_{x_{i-1}}^{x_i} \frac{x - x_{i-1}}{h} f(x)\,\mathrm{d}x + \int_{x_i}^{x_{i+1}} \left(1 - \frac{x - x_i}{h}\right) f(x)\,\mathrm{d}x\,. \tag{65}$$

We need a specific $f(x)$ function to compute these integrals. With $f(x) = x(1-x)$ and two equal-sized elements in $\Omega = [0,1]$, one gets

$$A = \frac{h}{6}\left(\begin{array}{ccc} 2 & 1 & 0\\ 1 & 4 & 1\\ 0 & 1 & 2 \end{array}\right),\quad b = \frac{h^2}{12}\left(\begin{array}{c} 2-h\\ 12-14h\\ 10-17h \end{array}\right).$$

The solution becomes

$$c_0 = \frac{h^2}{6},\quad c_1 = h - \frac{5}{6}h^2,\quad c_2 = 2h - \frac{23}{6}h^2\,.$$

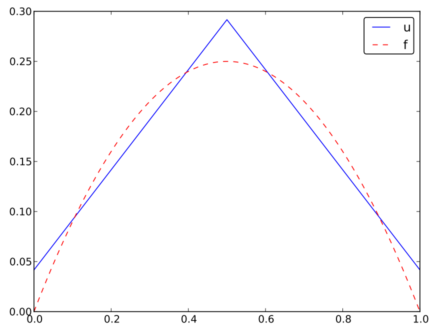
The resulting function

$$u(x) = c_0\varphi_0(x) + c_1\varphi_1(x) + c_2\varphi_2(x)$$

is displayed in Figure 27 (left). Doubling the number of elements to four leads to the improved approximation in the right part of Figure 27.

3.7 Assembly of elementwise computations

Our integral computations so far have been straightforward. However, with higher-degree polynomials and in higher dimensions (2D and 3D), integrating in



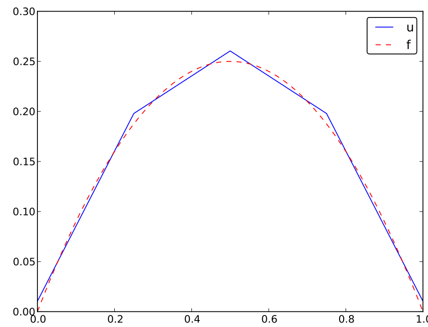


Figure 27: Least squares approximation of a parabola using 2 (left) and 4 (right) P1 elements.

the physical domain gets increasingly complicated. Instead, integrating over one element at a time, and transforming each element to a common standardized geometry in a new reference coordinate system, is technically easier. Almost all computer codes employ a finite element algorithm that calculates the linear system by integrating over one element at a time. We shall therefore explain this algorithm next. The amount of details might be overwhelming during a first reading, but once all those details are done right, one has a general finite element algorithm that can be applied to all sorts of elements, in any space dimension, no matter how geometrically complicated the domain is.

The element matrix. We start by splitting the integral over Ω into a sum of contributions from each element:

$$A_{i,j} = \int_\Omega \varphi_i\varphi_j \,\mathrm{d}x = \sum_e A_{i,j}^{(e)},\quad A_{i,j}^{(e)} = \int_{\Omega^{(e)}} \varphi_i\varphi_j \,\mathrm{d}x\,. \tag{66}$$

Now, $A_{i,j}^{(e)} \neq 0$, if and only if, i and j are nodes in element e (look at Figure 25 to realize this property, but the result also holds for all types of elements). Introduce $i = q(e, r)$ as the mapping of local node number r in element e to the global node number i. This is just a short mathematical notation for the expression `i=elements[e][r]` in a program. Let r and s be the local node numbers corresponding to the global node numbers $i = q(e, r)$ and $j = q(e, s)$. With d nodes per element, all the nonzero matrix entries in $A_{i,j}^{(e)}$ arise from the integrals involving basis functions with indices corresponding to the global node numbers in element number e:

$$\int_{\Omega^{(e)}} \varphi_{q(e,r)}\varphi_{q(e,s)} \,\mathrm{d}x,\quad r, s = 0, \ldots, d\,.$$

These contributions can be collected in a $(d+1)\times(d+1)$ matrix known as the *element matrix*. Let $I_d = \{0, \ldots, d\}$ be the valid indices of r and s. We introduce the notation

$$\tilde{A}^{(e)} = \{\tilde{A}^{(e)}_{r,s}\}, \quad r,s \in I_d,$$

for the element matrix. For P1 elements ($d = 1$) we have

$$\tilde{A}^{(e)} = \left[\begin{array}{cc} \tilde{A}^{(e)}_{0,0} & \tilde{A}^{(e)}_{0,1} \\ \tilde{A}^{(e)}_{1,0} & \tilde{A}^{(e)}_{1,1} \end{array}\right].$$

while P2 elements have a 3×3 element matrix:

$$\tilde{A}^{(e)} = \left[\begin{array}{ccc} \tilde{A}^{(e)}_{0,0} & \tilde{A}^{(e)}_{0,1} & \tilde{A}^{(e)}_{0,2} \\ \tilde{A}^{(e)}_{1,0} & \tilde{A}^{(e)}_{1,1} & \tilde{A}^{(e)}_{1,2} \\ \tilde{A}^{(e)}_{2,0} & \tilde{A}^{(e)}_{2,1} & \tilde{A}^{(e)}_{2,2} \end{array}\right].$$

Assembly of element matrices. Given the numbers $\tilde{A}^{(e)}_{r,s}$, we should, according to (66), add the contributions to the global coefficient matrix by

$$A_{q(e,r),q(e,s)} := A_{q(e,r),q(e,s)} + \tilde{A}^{(e)}_{r,s}, \quad r,s \in I_d\,. \tag{67}$$

This process of adding in elementwise contributions to the global matrix is called *finite element assembly* or simply *assembly*.

Figure 28 illustrates how element matrices for elements with two nodes are added into the global matrix. More specifically, the figure shows how the element matrix associated with elements 1 and 2 assembled, assuming that global nodes are numbered from left to right in the domain. With regularly numbered P3 elements, where the element matrices have size 4×4, the assembly of elements 1 and 2 are sketched in Figure 29.

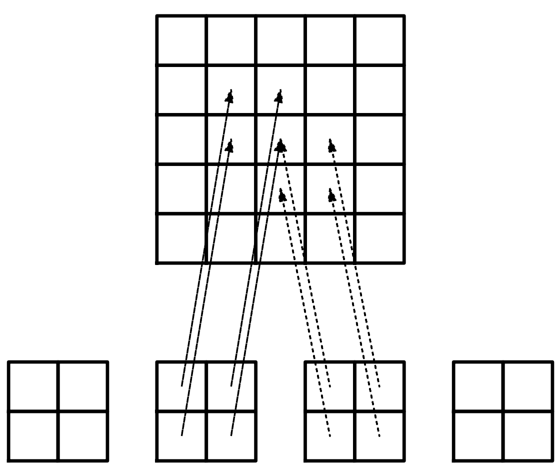


Figure 28: Illustration of matrix assembly: regularly numbered P1 elements.

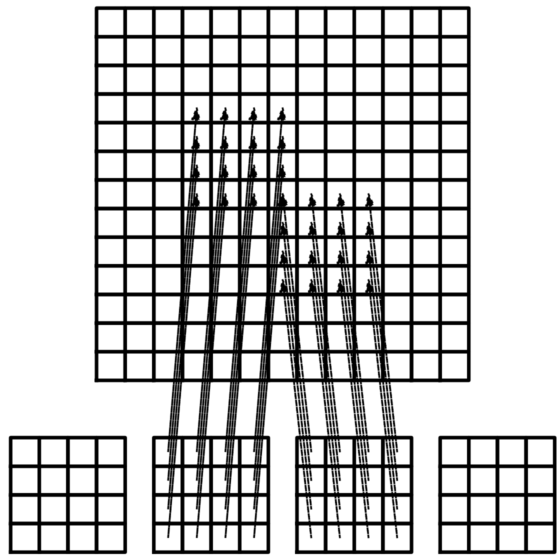


Figure 29: Illustration of matrix assembly: regularly numbered P3 elements.

Assembly of irregularly numbered elements and nodes. After assembly of element matrices corresponding to regularly numbered elements and nodes are understood, it is wise to study the assembly process for irregularly numbered elements and nodes. Figure 19 shows a mesh where the `elements` array, or $q(e,r)$ mapping in mathematical notation, is given as

```
elements = [[2, 1], [4, 5], [0, 4], [3, 0], [5, 2]]
```

The associated assembly of element matrices 1 and 2 is sketched in Figure 30.

We have created animations to illustrate the assembly of P1 and P3 elements with regular numbering as well as P1 elements with irregular numbering. The reader is encouraged to develop a "geometric" understanding of how element matrix entries are added to the global matrix. This understanding is crucial for hand computations with the finite element method.

The element vector. The right-hand side of the linear system is also computed elementwise:

$$b_i = \int_\Omega f(x)\varphi_i(x)\,\mathrm{d}x = \sum_e b_i^{(e)}, \quad b_i^{(e)} = \int_{\Omega^{(e)}} f(x)\varphi_i(x)\,\mathrm{d}x\,. \tag{68}$$

We observe that $b_i^{(e)} \neq 0$ if and only if global node i is a node in element e (look at Figure 26 to realize this property). With d nodes per element we can collect the $d+1$ nonzero contributions $b_i^{(e)}$, for $i = q(e,r)$, $r \in I_d$, in an *element vector*

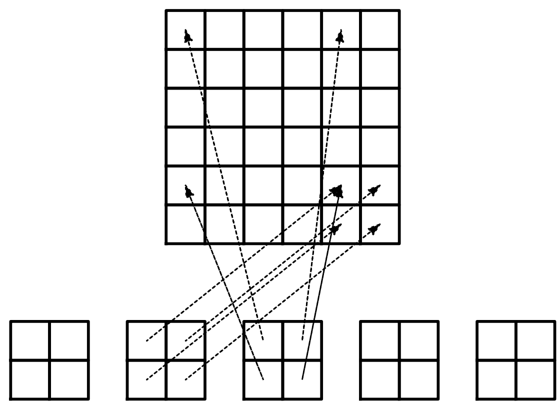


Figure 30: Illustration of matrix assembly: irregularly numbered P1 elements.

$$\tilde{b}_r^{(e)} = \{\tilde{b}_r^{(e)}\}, \quad r \in I_d\,.$$

These contributions are added to the global right-hand side by an assembly process similar to that for the element matrices:

$$b_{q(e,r)} := b_{q(e,r)} + \tilde{b}_r^{(e)}, \quad r \in I_d\,. \tag{69}$$

3.8 Mapping to a reference element

Instead of computing the integrals

$$\tilde{A}_{r,s}^{(e)} = \int_{\Omega^{(e)}} \varphi_{q(e,r)}(x)\varphi_{q(e,s)}(x)\,\mathrm{d}x$$

over some element $\Omega^{(e)} = [x_L, x_R]$ in the physical coordinate system, it turns out that it is considerably easier and more convenient to map the element domain $[x_L, x_R]$ to a standardized reference element domain $[-1, 1]$ and compute all integrals over the same domain $[-1, 1]$. We have now introduced x_L and x_R as the left and right boundary points of an arbitrary element. With a natural, regular numbering of nodes and elements from left to right through the domain, we have $x_L = x_e$ and $x_R = x_{e+1}$ for P1 elements.

The coordinate transformation. Let $X \in [-1, 1]$ be the coordinate in the reference element. A linear mapping, also known as an affine mapping, from X to x can be written

$$x = \frac{1}{2}(x_L + x_R) + \frac{1}{2}(x_R - x_L)X\,. \tag{70}$$

This relation can alternatively be expressed as

$$x = x_m + \frac{1}{2}hX, \tag{71}$$

where we have introduced the element midpoint $x_m = (x_L + x_R)/2$ and the element length $h = x_R - x_L$.

Formulas for the element matrix and vector entries. Integrating on the reference element is a matter of just changing the integration variable from x to X. Let

$$\tilde{\varphi}_r(X) = \varphi_{q(e,r)}(x(X)) \tag{72}$$

be the basis function associated with local node number r in the reference element. Switching from x to X as integration variable, using the rules from calculus, results in

$$\tilde{A}^{(e)}_{r,s} = \int_{\Omega^{(e)}} \varphi_{q(e,r)}(x)\varphi_{q(e,s)}(x)\,\mathrm{d}x = \int_{-1}^{1} \tilde{\varphi}_r(X)\tilde{\varphi}_s(X)\frac{\mathrm{d}x}{\mathrm{d}X}\,\mathrm{d}X\,. \tag{73}$$

In 2D and 3D, $\mathrm{d}x$ is transformed to $\det J\,\mathrm{d}X$, where J is the Jacobian of the mapping from x to X. In 1D, $\det J\,\mathrm{d}X = \mathrm{d}x/\mathrm{d}X = h/2$.To obtain a uniform notation for 1D, 2D, and 3D problems we therefore replace $\mathrm{d}x/\mathrm{d}X$ by $\det J$ already now. The integration over the reference element is then written as

$$\tilde{A}^{(e)}_{r,s} = \int_{-1}^{1} \tilde{\varphi}_r(X)\tilde{\varphi}_s(X)\det J\;\mathrm{d}X\,. \tag{74}$$

The corresponding formula for the element vector entries becomes

$$\tilde{b}^{(e)}_r = \int_{\Omega^{(e)}} f(x)\varphi_{q(e,r)}(x)\,\mathrm{d}x = \int_{-1}^{1} f(x(X))\tilde{\varphi}_r(X)\det J\;\mathrm{d}X\,. \tag{75}$$

Why reference elements?

The great advantage of using reference elements is that the formulas for the basis functions, $\tilde{\varphi}_r(X)$, are the same for all elements and independent of the element geometry (length and location in the mesh). The geometric information is "factored out" in the simple mapping formula and the associated $\det J$ quantity. Also, the integration domain is the same for all elements. All these features contribute to simplify computer codes and make them more general.

Formulas for local basis functions. The $\tilde{\varphi}_r(x)$ functions are simply the Lagrange polynomials defined through the local nodes in the reference element. For $d = 1$ and two nodes per element, we have the linear Lagrange polynomials

$$\tilde{\varphi}_0(X) = \frac{1}{2}(1 - X) \tag{76}$$

$$\tilde{\varphi}_1(X) = \frac{1}{2}(1 + X) \tag{77}$$

Quadratic polynomials, $d = 2$, have the formulas

$$\tilde{\varphi}_0(X) = \frac{1}{2}(X - 1)X \tag{78}$$

$$\tilde{\varphi}_1(X) = 1 - X^2 \tag{79}$$

$$\tilde{\varphi}_2(X) = \frac{1}{2}(X + 1)X \tag{80}$$

In general,

$$\tilde{\varphi}_r(X) = \prod_{s=0,s\neq r}^{d} \frac{X - X_{(s)}}{X_{(r)} - X_{(s)}}, \tag{81}$$

where $X_{(0)}, \ldots, X_{(d)}$ are the coordinates of the local nodes in the reference element. These are normally uniformly spaced: $X_{(r)} = -1 + 2r/d$, $r \in I_d$.

3.9 Example: Integration over a reference element

To illustrate the concepts from the previous section in a specific example, we now consider calculation of the element matrix and vector for a specific choice of d and $f(x)$. A simple choice is $d = 1$ (P1 elements) and $f(x) = x(1 - x)$ on $\Omega = [0, 1]$. We have the general expressions (74) and (75) for $\tilde{A}^{(e)}_{r,s}$ and $\tilde{b}^{(e)}_r$. Writing these out for the choices (76) and (77), and using that $\det J = h/2$, we can do the following calculations of the element matrix entries:

$$
\begin{aligned}
\tilde{A}^{(e)}_{0,0} &= \int_{-1}^{1} \tilde{\varphi}_0(X)\tilde{\varphi}_0(X)\frac{h}{2}\,\mathrm{d}X \\
&= \int_{-1}^{1} \frac{1}{2}(1-X)\frac{1}{2}(1-X)\frac{h}{2}\,\mathrm{d}X = \frac{h}{8}\int_{-1}^{1}(1-X)^2\,\mathrm{d}X = \frac{h}{3}, \qquad (82)\\
\tilde{A}^{(e)}_{1,0} &= \int_{-1}^{1} \tilde{\varphi}_1(X)\tilde{\varphi}_0(X)\frac{h}{2}\,\mathrm{d}X \\
&= \int_{-1}^{1} \frac{1}{2}(1+X)\frac{1}{2}(1-X)\frac{h}{2}\,\mathrm{d}X = \frac{h}{8}\int_{-1}^{1}(1-X^2)\,\mathrm{d}X = \frac{h}{6}, \qquad (83)\\
\tilde{A}^{(e)}_{0,1} &= \tilde{A}^{(e)}_{1,0}, \qquad (84)\\
\tilde{A}^{(e)}_{1,1} &= \int_{-1}^{1} \tilde{\varphi}_1(X)\tilde{\varphi}_1(X)\frac{h}{2}\,\mathrm{d}X \\
&= \int_{-1}^{1} \frac{1}{2}(1+X)\frac{1}{2}(1+X)\frac{h}{2}\,\mathrm{d}X = \frac{h}{8}\int_{-1}^{1}(1+X)^2\,\mathrm{d}X = \frac{h}{3}\,. \qquad (85)
\end{aligned}
$$

The corresponding entries in the element vector becomes

$$
\begin{aligned}
\tilde{b}^{(e)}_{0} &= \int_{-1}^{1} f(x(X))\tilde{\varphi}_0(X)\frac{h}{2}\,\mathrm{d}X \\
&= \int_{-1}^{1} (x_m + \frac{1}{2}hX)(1-(x_m+\frac{1}{2}hX))\frac{1}{2}(1-X)\frac{h}{2}\,\mathrm{d}X \\
&= -\frac{1}{24}h^3 + \frac{1}{6}h^2x_m - \frac{1}{12}h^2 - \frac{1}{2}hx_m^2 + \frac{1}{2}hx_m \qquad (86)\\
\tilde{b}^{(e)}_{1} &= \int_{-1}^{1} f(x(X))\tilde{\varphi}_1(X)\frac{h}{2}\,\mathrm{d}X \\
&= \int_{-1}^{1} (x_m + \frac{1}{2}hX)(1-(x_m+\frac{1}{2}hX))\frac{1}{2}(1+X)\frac{h}{2}\,\mathrm{d}X \\
&= -\frac{1}{24}h^3 - \frac{1}{6}h^2x_m + \frac{1}{12}h^2 - \frac{1}{2}hx_m^2 + \frac{1}{2}hx_m\,. \qquad (87)
\end{aligned}
$$

In the last two expressions we have used the element midpoint x_m.

Integration of lower-degree polynomials above is tedious, and higher-degree polynomials involve much more algebra, but `sympy` may help. For example, we can easily calculate (82), (83), and (86) by

```
>>> import sympy as sym
>>> x, x_m, h, X = sym.symbols('x x_m h X')
>>> sym.integrate(h/8*(1-X)**2, (X, -1, 1))
h/3
>>> sym.integrate(h/8*(1+X)*(1-X), (X, -1, 1))
h/6
>>> x = x_m + h/2*X
>>> b_0 = sym.integrate(h/4*x*(1-x)*(1-X), (X, -1, 1))
```

```
>>> print b_0
-h**3/24 + h**2*x_m/6 - h**2/12 - h*x_m**2/2 + h*x_m/2
```

4 Implementation

Based on the experience from the previous example, it makes sense to write some code to automate the analytical integration process for any choice of finite element basis functions. In addition, we can automate the assembly process and the solution of the linear system. Another advantage is that the code for these purposes document all details of all steps in the finite element computational machinery. The complete code can be found in the module file `fe_approx1D.py`.

4.1 Integration

First we need a Python function for defining $\tilde{\varphi}_r(X)$ in terms of a Lagrange polynomial of degree `d`:

```
import sympy as sym
import numpy as np

def basis(d, point_distribution='uniform', symbolic=False):
    """
    Return all local basis function phi as functions of the
    local point X in a 1D element with d+1 nodes.
    If symbolic=True, return symbolic expressions, else
    return Python functions of X.
    point_distribution can be 'uniform' or 'Chebyshev'.
    """
    X = sym.symbols('X')
    if d == 0:
        phi_sym = [1]
    else:
        if point_distribution == 'uniform':
            if symbolic:
                # Compute symbolic nodes
                h = sym.Rational(1, d)  # node spacing
                nodes = [2*i*h - 1 for i in range(d+1)]
            else:
                nodes = np.linspace(-1, 1, d+1)
        elif point_distribution == 'Chebyshev':
            # Just numeric nodes
            nodes = Chebyshev_nodes(-1, 1, d)

        phi_sym = [Lagrange_polynomial(X, r, nodes)
                   for r in range(d+1)]
    # Transform to Python functions
    phi_num = [sym.lambdify([X], phi_sym[r]) for r in range(d+1)]
    return phi_sym if symbolic else phi_num

def Lagrange_polynomial(x, i, points):
    p = 1
    for k in range(len(points)):
        if k != i:
            p *= (x - points[k])/(points[i] - points[k])
    return p
```

Observe how we construct the `phi_sym` list to be symbolic expressions for $\tilde{\varphi}_r(X)$ with `X` as a `Symbol` object from `sympy`. Also note that the `Lagrange_polynomial` function (here simply copied from Section 2.7) works with both symbolic and numeric variables.

Now we can write the function that computes the element matrix with a list of symbolic expressions for φ_r (`phi = basis(d, symbolic=True)`):

```
def element_matrix(phi, Omega_e, symbolic=True):
    n = len(phi)
    A_e = sym.zeros((n, n))
    X = sym.Symbol('X')
    if symbolic:
        h = sym.Symbol('h')
    else:
        h = Omega_e[1] - Omega_e[0]
    detJ = h/2  # dx/dX
    for r in range(n):
        for s in range(r, n):
            A_e[r,s] = sym.integrate(phi[r]*phi[s]*detJ, (X, -1, 1))
            A_e[s,r] = A_e[r,s]
    return A_e
```

In the symbolic case (`symbolic` is `True`), we introduce the element length as a symbol `h` in the computations. Otherwise, the real numerical value of the element interval `Omega_e` is used and the final matrix elements are numbers, not symbols. This functionality can be demonstrated:

```
>>> from fe_approx1D import *
>>> phi = basis(d=1, symbolic=True)
>>> phi
[-X/2 + 1/2, X/2 + 1/2]
>>> element_matrix(phi, Omega_e=[0.1, 0.2], symbolic=True)
[h/3, h/6]
[h/6, h/3]
>>> element_matrix(phi, Omega_e=[0.1, 0.2], symbolic=False)
[0.0333333333333333, 0.0166666666666667]
[0.0166666666666667, 0.0333333333333333]
```

The computation of the element vector is done by a similar procedure:

```
def element_vector(f, phi, Omega_e, symbolic=True):
    n = len(phi)
    b_e = sym.zeros((n, 1))
    # Make f a function of X
    X = sym.Symbol('X')
    if symbolic:
        h = sym.Symbol('h')
    else:
        h = Omega_e[1] - Omega_e[0]
    x = (Omega_e[0] + Omega_e[1])/2 + h/2*X  # mapping
    f = f.subs('x', x)  # substitute mapping formula for x
    detJ = h/2  # dx/dX
    for r in range(n):
        b_e[r] = sym.integrate(f*phi[r]*detJ, (X, -1, 1))
    return b_e
```

Here we need to replace the symbol `x` in the expression for `f` by the mapping formula such that `f` can be integrated in terms of X, cf. the formula $\tilde{b}_r^{(e)} = \int_{-1}^{1} f(x(X))\tilde{\varphi}_r(X)\frac{h}{2}\,\mathrm{d}X$.

The integration in the element matrix function involves only products of polynomials, which `sympy` can easily deal with, but for the right-hand side `sympy` may face difficulties with certain types of expressions `f`. The result of the integral is then an `Integral` object and not a number or expression as when symbolic integration is successful. It may therefore be wise to introduce a fall back on numerical integration. The symbolic integration can also spend considerable time before reaching an unsuccessful conclusion, so we may also introduce a parameter `symbolic` to turn symbolic integration on and off:

```
def element_vector(f, phi, Omega_e, symbolic=True):
        ...
        if symbolic:
            I = sym.integrate(f*phi[r]*detJ, (X, -1, 1))
        if not symbolic or isinstance(I, sym.Integral):
            h = Omega_e[1] - Omega_e[0]  # Ensure h is numerical
            detJ = h/2
            integrand = sym.lambdify([X], f*phi[r]*detJ)
            I = sym.mpmath.quad(integrand, [-1, 1])
        b_e[r] = I
        ...
```

Numerical integration requires that the symbolic integrand is converted to a plain Python function (`integrand`) and that the element length `h` is a real number.

4.2 Linear system assembly and solution

The complete algorithm for computing and assembling the elementwise contributions takes the following form

```
def assemble(nodes, elements, phi, f, symbolic=True):
    N_n, N_e = len(nodes), len(elements)
    if symbolic:
        A = sym.zeros((N_n, N_n))
        b = sym.zeros((N_n, 1))    # note: (N_n, 1) matrix
    else:
        A = np.zeros((N_n, N_n))
        b = np.zeros(N_n)
    for e in range(N_e):
        Omega_e = [nodes[elements[e][0]], nodes[elements[e][-1]]]

        A_e = element_matrix(phi, Omega_e, symbolic)
        b_e = element_vector(f, phi, Omega_e, symbolic)

        for r in range(len(elements[e])):
            for s in range(len(elements[e])):
                A[elements[e][r],elements[e][s]] += A_e[r,s]
            b[elements[e][r]] += b_e[r]
    return A, b
```

The `nodes` and `elements` variables represent the finite element mesh as explained earlier.

Given the coefficient matrix `A` and the right-hand side `b`, we can compute the coefficients $\{c_j\}_{j\in\mathcal{I}_s}$ in the expansion $u(x)=\sum_j c_j\varphi_j$ as the solution vector `c` of the linear system:

```
if symbolic:
    c = A.LUsolve(b)
else:
    c = np.linalg.solve(A, b)
```

When `A` and `b` are `sympy` arrays, the solution procedure implied by `A.LUsolve` is symbolic. Otherwise, `A` and `b` are `numpy` arrays and a standard numerical solver is called. The symbolic version is suited for small problems only (small N values) since the calculation time becomes prohibitively large otherwise. Normally, the symbolic *integration* will be more time consuming in small problems than the symbolic *solution* of the linear system.

4.3 Example on computing symbolic approximations

We can exemplify the use of `assemble` on the computational case from Section 3.6 with two P1 elements (linear basis functions) on the domain $\Omega=[0,1]$. Let us first work with a symbolic element length:

```
>>> h, x = sym.symbols('h x')
>>> nodes = [0, h, 2*h]
>>> elements = [[0, 1], [1, 2]]
>>> phi = basis(d=1, symbolic=True)
>>> f = x*(1-x)
>>> A, b = assemble(nodes, elements, phi, f, symbolic=True)
>>> A
[h/3,   h/6,   0]
[h/6, 2*h/3, h/6]
[  0,   h/6, h/3]
>>> b
[     h**2/6 - h**3/12]
[      h**2 - 7*h**3/6]
[5*h**2/6 - 17*h**3/12]
>>> c = A.LUsolve(b)
>>> c
[                           h**2/6]
[12*(7*h**2/12 - 35*h**3/72)/(7*h)]
[  7*(4*h**2/7 - 23*h**3/21)/(2*h)]
```

4.4 Using interpolation instead of least squares

As an alternative to the least squares formulation, we may compute the `c` vector based on the interpolation method from Section 2.10, using finite element basis functions. Choosing the nodes as interpolation points, the method can be written as

$$u(x_i)=\sum_{j\in\mathcal{I}_s} c_j\varphi_j(x_i)=f(x_i),\quad i\in\mathcal{I}_s\,.$$

The coefficient matrix $A_{i,j} = \varphi_j(x_i)$ becomes the identity matrix because basis function number j vanishes at all nodes, except node i: $\varphi_j(x_i) = \delta_{ij}$. Therefore, $c_i = f(x_i)$.

The associated sympy calculations are

```
>>> fn = sym.lambdify([x], f)
>>> c = [fn(xc) for xc in nodes]
>>> c
[0, h*(1 - h), 2*h*(1 - 2*h)]
```

These expressions are much simpler than those based on least squares or projection in combination with finite element basis functions. However, which of the two methods that is most appropriate for a given task is problem-dependent, so we need both methods in our toolbox.

4.5 Example on computing numerical approximations

The numerical computations corresponding to the symbolic ones in Section 4.3 (still done by `sympy` and the `assemble` function) go as follows:

```
>>> nodes = [0, 0.5, 1]
>>> elements = [[0, 1], [1, 2]]
>>> phi = basis(d=1, symbolic=True)
>>> x = sym.Symbol('x')
>>> f = x*(1-x)
>>> A, b = assemble(nodes, elements, phi, f, symbolic=False)
>>> A
[ 0.166666666666667, 0.0833333333333333,                  0]
[0.0833333333333333,  0.333333333333333, 0.0833333333333333]
[                 0, 0.0833333333333333,  0.166666666666667]
>>> b
[          0.03125]
[0.104166666666667]
[          0.03125]
>>> c = A.LUsolve(b)
>>> c
[0.0416666666666666]
[ 0.291666666666667]
[0.0416666666666666]
```

The `fe_approx1D` module contains functions for generating the `nodes` and `elements` lists for equal-sized elements with any number of nodes per element. The coordinates in `nodes` can be expressed either through the element length symbol `h` (`symbolic=True`) or by real numbers (`symbolic=False`):

```
nodes, elements = mesh_uniform(N_e=10, d=3, Omega=[0,1],
                               symbolic=True)
```

There is also a function

```
def approximate(f, symbolic=False, d=1, N_e=4, filename='tmp.pdf'):
```

which computes a mesh with `N_e` elements, basis functions of degree `d`, and approximates a given symbolic expression `f` by a finite element expansion $u(x) =$

$\sum_j c_j\varphi_j(x)$. When `symbolic` is `False`, $u(x)=\sum_j c_j\varphi_j(x)$ can be computed at a (large) number of points and plotted together with $f(x)$. The construction of u points from the solution vector `c` is done elementwise by evaluating $\sum_r c_r\tilde{\varphi}_r(X)$ at a (large) number of points in each element in the local coordinate system, and the discrete (x,u) values on each element are stored in separate arrays that are finally concatenated to form a global array for x and for u. The details are found in the `u_glob` function in `fe_approx1D.py`.

4.6 The structure of the coefficient matrix

Let us first see how the global matrix looks like if we assemble symbolic element matrices, expressed in terms of `h`, from several elements:

```
>>> d=1; N_e=8; Omega=[0,1]  # 8 linear elements on [0,1]
>>> phi = basis(d)
>>> f = x*(1-x)
>>> nodes, elements = mesh_symbolic(N_e, d, Omega)
>>> A, b = assemble(nodes, elements, phi, f, symbolic=True)
>>> A
[h/3,   h/6,     0,     0,     0,     0,     0,     0,   0]
[h/6, 2*h/3,   h/6,     0,     0,     0,     0,     0,   0]
[  0,   h/6, 2*h/3,   h/6,     0,     0,     0,     0,   0]
[  0,     0,   h/6, 2*h/3,   h/6,     0,     0,     0,   0]
[  0,     0,     0,   h/6, 2*h/3,   h/6,     0,     0,   0]
[  0,     0,     0,     0,   h/6, 2*h/3,   h/6,     0,   0]
[  0,     0,     0,     0,     0,   h/6, 2*h/3,   h/6,   0]
[  0,     0,     0,     0,     0,     0,   h/6, 2*h/3, h/6]
[  0,     0,     0,     0,     0,     0,     0,   h/6, h/3]
```

The reader is encouraged to assemble the element matrices by hand and verify this result, as this exercise will give a hands-on understanding of what the assembly is about. In general we have a coefficient matrix that is tridiagonal:

$$A=\frac{h}{6}\left(\begin{array}{cccccccccc}
2 & 1 & 0 & \cdots & \cdots & \cdots & \cdots & \cdots & 0 \\
1 & 4 & 1 & \ddots & & & & & \vdots \\
0 & 1 & 4 & 1 & \ddots & & & & \vdots \\
\vdots & \ddots & & \ddots & \ddots & 0 & & & \vdots \\
\vdots & & \ddots & \ddots & \ddots & \ddots & \ddots & & \vdots \\
\vdots & & & 0 & 1 & 4 & 1 & \ddots & \vdots \\
\vdots & & & & \ddots & \ddots & \ddots & \ddots & 0 \\
\vdots & & & & & \ddots & 1 & 4 & 1 \\
0 & \cdots & \cdots & \cdots & \cdots & \cdots & 0 & 1 & 2
\end{array}\right) \tag{88}$$

The structure of the right-hand side is more difficult to reveal since it involves an assembly of elementwise integrals of $f(x(X))\tilde{\varphi}_r(X)h/2$, which obviously depend on the particular choice of $f(x)$. Numerical integration can give some insight into the nature of the right-hand side. For this purpose it is easier to look at the integration in x coordinates, which gives the general formula (65). For equal-sized elements of length h, we can apply the Trapezoidal rule at the global node points to arrive at

$$b_i = h\left(\frac{1}{2}\varphi_i(x_0)f(x_0) + \frac{1}{2}\varphi_i(x_N)f(x_N) + \sum_{j=1}^{N-1}\varphi_i(x_j)f(x_j)\right) \tag{89}$$

$$= \begin{cases} \frac{1}{2}hf(x_i), & i = 0 \text{ or } i = N, \\ hf(x_i), & 1 \leq i \leq N-1 \end{cases} \tag{90}$$

The reason for this simple formula is just that φ_i is either 0 or 1 at the nodes and 0 at all but one of them.

Going to P2 elements (`d=2`) leads to the element matrix

$$A^{(e)} = \frac{h}{30}\left(\begin{array}{ccc} 4 & 2 & -1 \\ 2 & 16 & 2 \\ -1 & 2 & 4 \end{array}\right) \tag{91}$$

and the following global matrix, assembled here from four elements:

$$A = \frac{h}{30}\left(\begin{array}{ccccccccc} 4 & 2 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 2 & 16 & 2 & 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & 2 & 8 & 2 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 2 & 16 & 2 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 2 & 8 & 2 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 2 & 16 & 2 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 2 & 8 & 2 & -1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 2 & 16 & 2 \\ 0 & 0 & 0 & 0 & 0 & 0 & -1 & 2 & 4 \end{array}\right) \tag{92}$$

In general, for i odd we have the nonzeroes

$$A_{i,i-2} = -1,\quad A_{i-1,i} = 2,\quad A_{i,i} = 8,\quad A_{i+1,i} = 2,\quad A_{i+2,i} = -1,$$

multiplied by $h/30$, and for i even we have the nonzeros

$$A_{i-1,i} = 2,\quad A_{i,i} = 16,\quad A_{i+1,i} = 2,$$

multiplied by $h/30$. The rows with odd numbers correspond to nodes at the element boundaries and get contributions from two neighboring elements in the assembly process, while the even numbered rows correspond to internal nodes in the elements where only one element contributes to the values in the global matrix.

4.7 Applications

With the aid of the `approximate` function in the `fe_approx1D` module we can easily investigate the quality of various finite element approximations to some given functions. Figure 31 shows how linear and quadratic elements approximate the polynomial $f(x) = x(1-x)^8$ on $\Omega = [0, 1]$, using equal-sized elements. The results arise from the program

```
import sympy as sym
from fe_approx1D import approximate
x = sym.Symbol('x')

approximate(f=x*(1-x)**8, symbolic=False, d=1, N_e=4)
approximate(f=x*(1-x)**8, symbolic=False, d=2, N_e=2)
approximate(f=x*(1-x)**8, symbolic=False, d=1, N_e=8)
approximate(f=x*(1-x)**8, symbolic=False, d=2, N_e=4)
```

The quadratic functions are seen to be better than the linear ones for the same value of N, as we increase N. This observation has some generality: higher degree is not necessarily better on a coarse mesh, but it is as we refine the mesh.

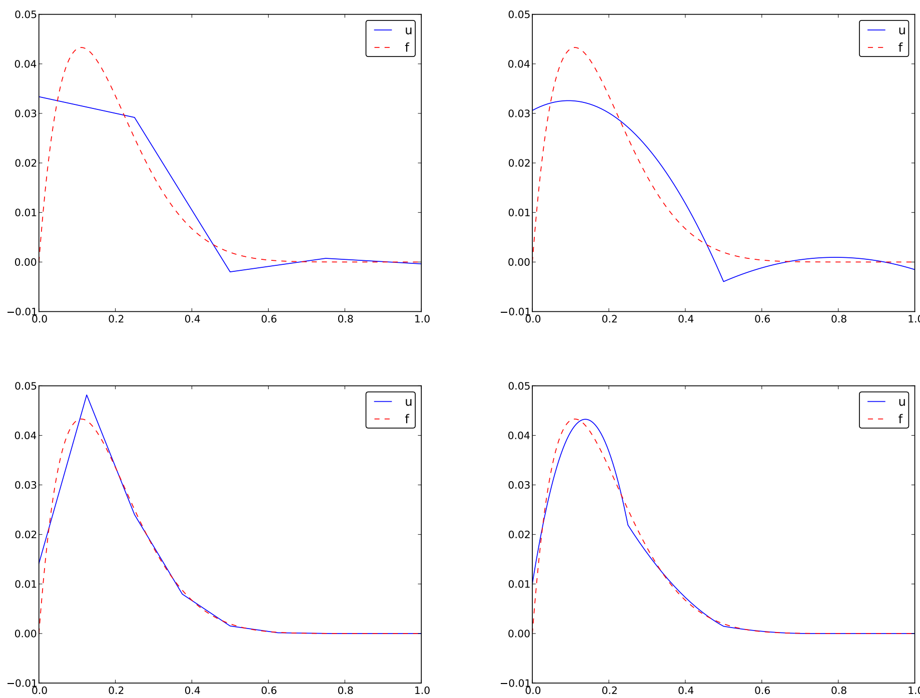


Figure 31: Comparison of the finite element approximations: 4 P1 elements with 5 nodes (upper left), 2 P2 elements with 5 nodes (upper right), 8 P1 elements with 9 nodes (lower left), and 4 P2 elements with 9 nodes (lower right).

4.8 Sparse matrix storage and solution

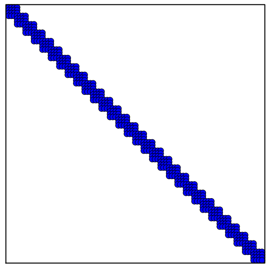
Some of the examples in the preceding section took several minutes to compute, even on small meshes consisting of up to eight elements. The main explanation for slow computations is unsuccessful symbolic integration: `sympy` may use a lot of energy on integrals like $\int f(x(X))\tilde{\varphi}_r(X)h/2\,\mathrm{d}x$ before giving up, and the program then resorts to numerical integration. Codes that can deal with a large number of basis functions and accept flexible choices of $f(x)$ should compute all integrals numerically and replace the matrix objects from `sympy` by the far more efficient array objects from `numpy`.

There is also another (potential) reason for slow code: the solution algorithm for the linear system performs much more work than necessary. Most of the matrix entries $A_{i,j}$ are zero, because $(\varphi_i, \varphi_j) = 0$ unless i and j are nodes in the same element. In 1D problems, we do not need to store or compute with these zeros when solving the linear system, but that requires solution methods adapted to the kind of matrices produced by the finite element approximations.

A matrix whose majority of entries are zeros, is known as a sparse matrix. Utilizing sparsity in software dramatically decreases the storage demands and the CPU-time needed to compute the solution of the linear system. This optimization is not very critical in 1D problems where modern computers can afford computing with all the zeros in the complete square matrix, but in 2D and especially in 3D, sparse matrices are fundamental for feasible finite element computations. One of the advantageous features of the finite element method is that it produces very sparse matrices. The reason is that the basis functions have local support such that the product of two basis functions, as typically met in integrals, is mostly zero.

Using a numbering of nodes and elements from left to right over a 1D domain, the assembled coefficient matrix has only a few diagonals different from zero. More precisely, $2d+1$ diagonals around the main diagonal are different from zero. With a different numbering of global nodes, say a random ordering, the diagonal structure is lost, but the number of nonzero elements is unaltered. Figures 32 and 33 exemplify sparsity patterns.

Figure 32: Matrix sparsity pattern for left-to-right numbering (left) and random numbering (right) of nodes in P1 elements.



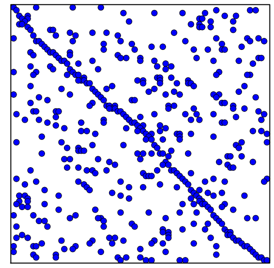


Figure 33: Matrix sparsity pattern for left-to-right numbering (left) and random numbering (right) of nodes in P3 elements.

The `scipy.sparse` library supports creation of sparse matrices and linear system solution.

- `scipy.sparse.diags` for matrix defined via diagonals
- `scipy.sparse.dok_matrix` for matrix incrementally defined via index pairs (i, j)

The `dok_matrix` object is most convenient for finite element computations. This sparse matrix format is called DOK, which stands for Dictionary Of Keys: the implementation is basically a dictionary (hash) with the entry indices `(i,j)` as keys.

Rather than declaring `A = np.zeros((N_n, N_n))`, a DOK sparse matrix is created by

```
import scipy.sparse
A = scipy.sparse.dok_matrix((N_n, N_n))
```

When there is any need to add or set some matrix entry `i,j`, just do

```
A[i,j]  = entry
# or
A[i,j] += entry
```

The indexing creates the matrix entry on the fly, and only the nonzero entries in the matrix will be stored.

To solve a system with right-hand side `b` (one-dimensional `numpy` array) with a sparse coefficient matrix `A`, we must use some kind of a sparse linear system solver. The safest choice is a method based on sparse Gaussian elimination:

```
import scipy.sparse.linalg
c = scipy.sparse.linalg.spsolve(A.tocsr(), b, use_umfpack=True)
```

The call `A.tocsr()` is not strictly needed (a warning is issued otherwise), but ensures that the solution algorithm can efficiently work with a copy of the sparse matrix in *Compressed Sparse Row* (CSR) format.

An advantage of the `scipy.sparse.diags` matrix over the DOK format is that the former allows vectorized assignment to the matrix. Vectorization is possible for approximation problems when all elements are of the same type. However, when solving differential equations, vectorization is much more difficult. It also appears that the DOK sparse matrix format available in the `scipy.sparse` package is fast enough even for big 1D problems on today's laptops, so the need for improving efficiency occurs in 2D and 3D problems, but then the complexity of the mesh favors the DOK format.

5 Comparison of finite element and finite difference approximations

The previous sections on approximating f by a finite element function u utilize the projection/Galerkin or least squares approaches to minimize the approximation error. We may, alternatively, use the collocation/interpolation method as described in Section 4.4. Here we shall compare these three approaches with what one does in the finite difference method when representing a given function on a mesh.

5.1 Finite difference approximation of given functions

Approximating a given function $f(x)$ on a mesh in a finite difference context will typically just sample f at the mesh points. If u_i is the value of the approximate u at the mesh point x_i, we have $u_i = f(x_i)$. The collocation/interpolation method using finite element basis functions gives exactly the same representation, as shown Section 4.4,

$$u(x_i) = c_i = f(x_i)\,.$$

How does a finite element Galerkin or least squares approximation differ from this straightforward interpolation of f? This is the question to be addressed next. We now limit the scope to P1 elements since this is the element type that gives formulas closest to those arising in the finite difference method.

5.2 Finite difference interpretation of a finite element approximation

The linear system arising from a Galerkin or least squares approximation reads in general

$$\sum_{j\in\mathcal{I}_s} c_j(\psi_i,\psi_j) = (f,\psi_i),\quad i\in\mathcal{I}_s\,.$$

In the finite element approximation we choose $\psi_i = \varphi_i$. With φ_i corresponding to P1 elements and a uniform mesh of element length h we have in Section 3.6 calculated the matrix with entries (φ_i,φ_j). Equation number i reads

$$\frac{h}{6}(u_{i-1} + 4u_i + u_{i+1}) = (f, \varphi_i)\,. \tag{93}$$

The first and last equation, corresponding to $i = 0$ and $i = N$ are slightly different, see Section 4.6.

The finite difference counterpart to (93) is just $u_i = f_i$ as explained in Section 5.1. To easier compare this result to the finite element approach to approximating functions, we can rewrite the left-hand side of (93) as

$$h(u_i + \frac{1}{6}(u_{i-1} - 2u_i + u_{i+1}))\,. \tag{94}$$

Thinking in terms of finite differences, we can write this expression using finite difference operator notation:

$$[h(u + \frac{h^2}{6}D_x D_x u)]_i,$$

which is nothing but the standard discretization of

$$h(u + \frac{h^2}{6}u'')\,.$$

Before interpreting the approximation procedure as solving a differential equation, we need to work out what the right-hand side is in the context of P1 elements. Since φ_i is the linear function that is 1 at x_i and zero at all other nodes, only the interval $[x_{i-1}, x_{i+1}]$ contribute to the integral on the right-hand side. This integral is naturally split into two parts according to (63):

$$(f, \varphi_i) = \int_{x_{i-1}}^{x_i} f(x)\frac{1}{h}(x - x_{i-1})\,\mathrm{d}x + \int_{x_i}^{x_{i+1}} f(x)(1 - \frac{1}{h}(x - x_i))\,\mathrm{d}x\,.$$

However, if f is not known we cannot do much else with this expression. It is clear that many values of f around x_i contribute to the right-hand side, not just the single point value $f(x_i)$ as in the finite difference method.

To proceed with the right-hand side, we can turn to numerical integration schemes. The Trapezoidal method for (f, φ_i), based on sampling the integrand $f\varphi_i$ at the node points $x_i = ih$ gives

$$(f, \varphi_i) = \int_\Omega f\varphi_i\,\mathrm{d}x \approx h\frac{1}{2}(f(x_0)\varphi_i(x_0) + f(x_N)\varphi_i(x_N)) + h\sum_{j=1}^{N-1} f(x_j)\varphi_i(x_j)\,.$$

Since φ_i is zero at all these points, except at x_i, the Trapezoidal rule collapses to one term:

$$(f, \varphi_i) \approx hf(x_i), \tag{95}$$

for $i=1,\ldots,N-1$, which is the same result as with collocation/interpolation, and of course the same result as in the finite difference method. For the end points $i=0$ and $i=N$ we get contribution from only one element so

$$(f,\varphi_i) \approx \frac{1}{2}hf(x_i), \quad i=0,\ i=N\,. \tag{96}$$

Simpson's rule with sample points also in the middle of the elements, at $x_{i+\frac{1}{2}}=(x_i+x_{i+1})/2$, can be written as

$$\int_\Omega g(x)\,\mathrm{d}x \approx \frac{\tilde{h}}{3}\left(g(x_0)+2\sum_{j=1}^{N-1}g(x_j)+4\sum_{j=0}^{N-1}g(x_{j+\frac{1}{2}})+f(x_{2N})\right),$$

where $\tilde{h}=h/2$ is the spacing between the sample points. Our integrand is $g=f\varphi_i$. For all the node points, $\varphi_i(x_j)=\delta_{ij}$, and therefore $\sum_{j=1}^{N-1}f(x_j)\varphi_i(x_j)=f(x_i)$. At the midpoints, $\varphi_i(x_{i\pm\frac{1}{2}})=1/2$ and $\varphi_i(x_{j+\frac{1}{2}})=0$ for $j>1$ and $j<i-1$. Consequently,

$$\sum_{j=0}^{N-1}f(x_{j+\frac{1}{2}})\varphi_i(x_{j+\frac{1}{2}})=\frac{1}{2}(fx_{j-\frac{1}{2}}+x_{j+\frac{1}{2}})\,.$$

When $1\leq i\leq N-1$ we then get

$$(f,\varphi_i)\approx\frac{h}{3}(f_{i-\frac{1}{2}}+f_i+f_{i+\frac{1}{2}})\,. \tag{97}$$

This result shows that, with Simpson's rule, the finite element method operates with the average of f over three points, while the finite difference method just applies f at one point. We may interpret this as a "smearing" or smoothing of f by the finite element method.

We can now summarize our findings. With the approximation of (f,φ_i) by the Trapezoidal rule, P1 elements give rise to equations that can be expressed as a finite difference discretization of

$$u+\frac{h^2}{6}u''=f, \quad u'(0)=u'(L)=0, \tag{98}$$

expressed with operator notation as

$$[u+\frac{h^2}{6}D_xD_xu=f]_i\,. \tag{99}$$

As $h\to 0$, the extra term proportional to u'' goes to zero, and the two methods are then equal.

With the Simpson's rule, we may say that we solve

$$[u+\frac{h^2}{6}D_xD_xu=\bar{f}]_i, \tag{100}$$

where $\bar{f}_i$ means the average $\frac{1}{3}(f_{i-1/2} + f_i + f_{i+1/2})$.

The extra term $\frac{h^2}{6}u''$ represents a smoothing effect: with just this term, we would find u by integrating f twice and thereby smooth f considerably. In addition, the finite element representation of f involves an average, or a smoothing, of f on the right-hand side of the equation system. If f is a noisy function, direct interpolation $u_i = f_i$ may result in a noisy u too, but with a Galerkin or least squares formulation and P1 elements, we should expect that u is smoother than f unless h is very small.

The interpretation that finite elements tend to smooth the solution is valid in applications far beyond approximation of 1D functions.

5.3 Making finite elements behave as finite differences

With a simple trick, using numerical integration, we can easily produce the result $u_i = f_i$ with the Galerkin or least square formulation with P1 elements. This is useful in many occasions when we deal with more difficult differential equations and want the finite element method to have properties like the finite difference method (solving standard linear wave equations is one primary example).

Computations in physical space. We have already seen that applying the Trapezoidal rule to the right-hand side (f, φ_i) simply gives f sampled at x_i. Using the Trapezoidal rule on the matrix entries $A_{i,j} = (\varphi_i, \varphi_j)$ involves a sum

$$\sum_k \varphi_i(x_k)\varphi_j(x_k),$$

but $\varphi_i(x_k) = \delta_{ik}$ and $\varphi_j(x_k) = \delta_{jk}$. The product $\varphi_i\varphi_j$ is then different from zero only when sampled at x_i and $i = j$. The Trapezoidal approximation to the integral is then

$$(\varphi_i, \varphi_j) \approx h, \quad i = j,$$

and zero if $i \neq j$. This means that we have obtained a diagonal matrix! The first and last diagonal elements, (φ_0, φ_0) and (φ_N, φ_N) get contribution only from the first and last element, respectively, resulting in the approximate integral value $h/2$. The corresponding right-hand side also has a factor $1/2$ for $i = 0$ and $i = N$. Therefore, the least squares or Galerkin approach with P1 elements and Trapezoidal integration results in

$$c_i = f_i, \quad i \in \mathcal{I}_s\,.$$

Simpsons's rule can be used to achieve a similar result for P2 elements, i.e, a diagonal coefficient matrix, but with the previously derived average of f on the right-hand side.

Elementwise computations. Identical results to those above will arise if we perform elementwise computations. The idea is to use the Trapezoidal rule on the reference element for computing the element matrix and vector. When assembled, the same equations $c_i = f(x_i)$ arise. Exercise 20 encourages you to carry out the details.

Terminology. The matrix with entries (φ_i, φ_j) typically arises from terms proportional to u in a differential equation where u is the unknown function. This matrix is often called the *mass matrix*, because in the early days of the finite element method, the matrix arose from the mass times acceleration term in Newton's second law of motion. Making the mass matrix diagonal by, e.g., numerical integration, as demonstrated above, is a widely used technique and is called *mass lumping*. In time-dependent problems it can sometimes enhance the numerical accuracy and computational efficiency of the finite element method. However, there are also examples where mass lumping destroys accuracy.

6 A generalized element concept

So far, finite element computing has employed the `nodes` and `element` lists together with the definition of the basis functions in the reference element. Suppose we want to introduce a piecewise constant approximation with one basis function $\tilde{\varphi}_0(x) = 1$ in the reference element, corresponding to a $\varphi_i(x)$ function that is 1 on element number i and zero on all other elements. Although we could associate the function value with a node in the middle of the elements, there are no nodes at the ends, and the previous code snippets will not work because we cannot find the element boundaries from the `nodes` list.

In order to get a richer space of finite element approximations, we need to revise the simple node and element concept presented so far and introduce a more powerful terminology. Much literature employs the definition of node and element introduced in the previous sections so it is important have this knowledge, besides being a good pedagogical background from understanding the extended element concept in the following.

6.1 Cells, vertices, and degrees of freedom

We now introduce *cells* as the subdomains $\Omega^{(e)}$ previously referred to as elements. The cell boundaries are denoted as *vertices*. The reason for this name is that cells are recognized by their vertices in 2D and 3D. We also define a set of *degrees of freedom* (dof), which are the quantities we aim to compute. The most common type of degree of freedom is the value of the unknown function u at some point. (For example, we can introduce nodes as before and say the degrees of freedom are the values of u at the nodes.) The basis functions are constructed so that they equal unity for one particular degree of freedom and zero for the rest. This property ensures that when we evaluate $u = \sum_j c_j \varphi_j$ for degree of freedom number i, we get $u = c_i$. Integrals are performed over cells, usually by mapping the cell of interest to a *reference cell*.

With the concepts of cells, vertices, and degrees of freedom we increase the decoupling of the geometry (cell, vertices) from the space of basis functions. We will associate different sets of basis functions with a cell. In 1D, all cells are intervals, while in 2D we can have cells that are triangles with straight sides, or any polygon, or in fact any two-dimensional geometry. Triangles and quadrilaterals are most common, though. The popular cell types in 3D are tetrahedra and hexahedra.

6.2 Extended finite element concept

The concept of a *finite element* is now

- a *reference cell* in a local reference coordinate system;
- a set of *basis functions* $\tilde{\varphi}_i$ defined on the cell;
- a set of *degrees of freedom* that uniquely determines the basis functions such that $\tilde{\varphi}_i = 1$ for degree of freedom number i and $\tilde{\varphi}_i = 0$ for all other degrees of freedom;
- a mapping between local and global degree of freedom numbers, here called the *dof map*;
- a geometric *mapping* of the reference cell onto the cell in the physical domain.

There must be a geometric description of a cell. This is trivial in 1D since the cell is an interval and is described by the interval limits, here called vertices. If the cell is $\Omega^{(e)} = [x_L, x_R]$, vertex 0 is x_L and vertex 1 is x_R. The reference cell in 1D is $[-1, 1]$ in the reference coordinate system X.

The expansion of u over one cell is often used:

$$u(x) = \tilde{u}(X) = \sum_r c_r \tilde{\varphi}_r(X), \quad x \in \Omega^{(e)},\ X \in [-1, 1], \tag{101}$$

where the sum is taken over the numbers of the degrees of freedom and c_r is the value of u for degree of freedom number r.

Our previous P1, P2, etc., elements are defined by introducing $d + 1$ equally spaced nodes in the reference cell and saying that the degrees of freedom are the $d + 1$ function values at these nodes. The basis functions must be 1 at one node and 0 at the others, and the Lagrange polynomials have exactly this property. The nodes can be numbered from left to right with associated degrees of freedom that are numbered in the same way. The degree of freedom mapping becomes what was previously represented by the `elements` lists. The cell mapping is the same affine mapping (70) as before.

6.3 Implementation

Implementationwise,

- we replace `nodes` by `vertices`;
- we introduce `cells` such that `cell[e][r]` gives the mapping from local vertex `r` in cell `e` to the global vertex number in `vertices`;
- we replace `elements` by `dof_map` (the contents are the same for Pd elements).

Consider the example from Section 3.1 where $\Omega = [0, 1]$ is divided into two cells, $\Omega^{(0)} = [0, 0.4]$ and $\Omega^{(1)} = [0.4, 1]$, as depicted in Figure 18. The vertices are $[0, 0.4, 1]$. Local vertex 0 and 1 are 0 and 0.4 in cell 0 and 0.4 and 1 in cell 1. A P2 element means that the degrees of freedom are the value of u at three equally spaced points (nodes) in each cell. The data structures become

```
vertices = [0, 0.4, 1]
cells = [[0, 1], [1, 2]]
dof_map = [[0, 1, 2], [2, 3, 4]]
```

If we would approximate f by piecewise constants, known as P0 elements, we simply introduce one point or node in an element, preferably $X = 0$, and define one degree of freedom, which is the function value at this node. Moreover, we set $\tilde{\varphi}_0(X) = 1$. The `cells` and `vertices` arrays remain the same, but `dof_map` is altered:

```
dof_map = [[0], [1]]
```

We use the `cells` and `vertices` lists to retrieve information on the geometry of a cell, while `dof_map` is the $q(e, r)$ mapping introduced earlier in the assembly of element matrices and vectors. For example, the `Omega_e` variable (representing the cell interval) in previous code snippets must now be computed as

```
Omega_e = [vertices[cells[e][0], vertices[cells[e][1]]
```

The assembly is done by

```
A[dof_map[e][r], dof_map[e][s]] += A_e[r,s]
b[dof_map[e][r]] += b_e[r]
```

We will hereafter drop the `nodes` and `elements` arrays and work exclusively with `cells`, `vertices`, and `dof_map`. The module `fe_approx1D_numint.py` now replaces the module `fe_approx1D` and offers similar functions that work with the new concepts:

```
from fe_approx1D_numint import *
x = sym.Symbol('x')
f = x*(1 - x)
N_e = 10
vertices, cells, dof_map = mesh_uniform(N_e, d=3, Omega=[0,1])
phi = [basis(len(dof_map[e])-1) for e in range(N_e)]
A, b = assemble(vertices, cells, dof_map, phi, f)
c = np.linalg.solve(A, b)
# Make very fine mesh and sample u(x) on this mesh for plotting
x_u, u = u_glob(c, vertices, cells, dof_map,
                resolution_per_element=51)
plot(x_u, u)
```

These steps are offered in the `approximate` function, which we here apply to see how well four P0 elements (piecewise constants) can approximate a parabola:

```
from fe_approx1D_numint import *
x=sym.Symbol("x")
for N_e in 4, 8:
    approximate(x*(1-x), d=0, N_e=N_e, Omega=[0,1])
```

Figure 34 shows the result.

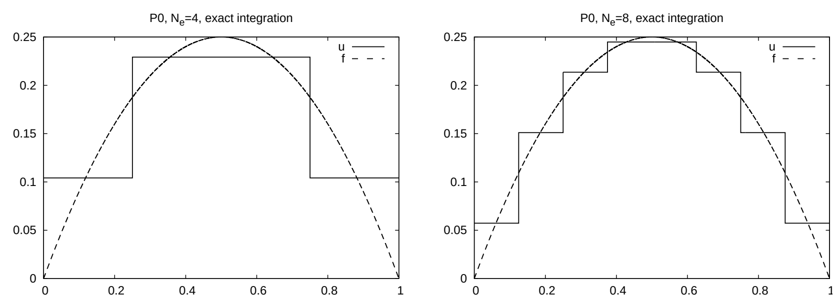


Figure 34: Approximation of a parabola by 4 (left) and 8 (right) P0 elements.

6.4 Computing the error of the approximation

So far we have focused on computing the coefficients c_j in the approximation $u(x) = \sum_j c_j\varphi_j$ as well as on plotting u and f for visual comparison. A more quantitative comparison needs to investigate the error $e(x) = f(x) - u(x)$. We mostly want a single number to reflect the error and use a norm for this purpose, usually the L^2 norm

$$||e||_{L^2} = \left(\int_\Omega e^2 \,\mathrm{d}x\right)^{1/2} .$$

Since the finite element approximation is defined for all $x \in \Omega$, and we are interested in how $u(x)$ deviates from $f(x)$ through all the elements, we can either integrate analytically or use an accurate numerical approximation. The latter is more convenient as it is a generally feasible and simple approach. The idea is to sample $e(x)$ at a large number of points in each element. The function `u_glob` in the `fe_approx1D_numint` module does this for $u(x)$ and returns an array `x` with coordinates and an array `u` with the u values:

```
x, u = u_glob(c, vertices, cells, dof_map,
              resolution_per_element=101)
e = f(x) - u
```

Let us use the Trapezoidal method to approximate the integral. Because different elements may have different lengths, the `x` array has a non-uniformly distributed set of coordinates. Also, the `u_glob` function works in an element by element fashion such that coordinates at the boundaries between elements appear twice. We therefore need to use a "raw" version of the Trapezoidal rule where we just add up all the trapezoids:

$$\int_\Omega g(x)\,\mathrm{d}x \approx \sum_{j=0}^{n-1} \frac{1}{2}(g(x_j) + g(x_{j+1}))(x_{j+1} - x_j),$$

if $x_0, \ldots, x_n$ are all the coordinates in `x`. In vectorized Python code,

```
g_x = g(x)
integral = 0.5*np.sum((g_x[:-1] + g_x[1:])*(x[1:] - x[:-1]))
```

Computing the L^2 norm of the error, here named `E`, is now achieved by

```
e2 = e**2
E = np.sqrt(0.5*np.sum((e2[:-1] + e2[1:])*(x[1:] - x[:-1]))
```

How does the error depend on h and d?

Theory and experiments show that the least squares or projection/Galerkin method in combination with Pd elements of equal length h has an error

$$||e||_{L^2} = Ch^{d+1}, \tag{102}$$

where C is a constant depending on f, but not on h or d.

6.5 Example: Cubic Hermite polynomials

The finite elements considered so far represent u as piecewise polynomials with discontinuous derivatives at the cell boundaries. Sometimes it is desirable to have continuous derivatives. A primary example is the solution of differential equations with fourth-order derivatives where standard finite element formulations lead to a need for basis functions with continuous first-order derivatives. The most common type of such basis functions in 1D is the so-called cubic Hermite polynomials. The construction of such polynomials, as explained next, will further exemplify the concepts of a cell, vertex, degree of freedom, and dof map.

Given a reference cell $[-1,1]$, we seek cubic polynomials with the values of the *function* and its *first-order derivative* at $X=-1$ and $X=1$ as the four degrees of freedom. Let us number the degrees of freedom as

- 0: value of function at $X=-1$
- 1: value of first derivative at $X=-1$
- 2: value of function at $X=1$
- 3: value of first derivative at $X=1$

By having the derivatives as unknowns, we ensure that the derivative of a basis function in two neighboring elements is the same at the node points.

The four basis functions can be written in a general form

$$\tilde{\varphi}_i(X)=\sum_{j=0}^{3} C_{i,j}X^j,$$

with four coefficients $C_{i,j}$, $j=0,1,2,3$, to be determined for each i. The constraints that basis function number i must be 1 for degree of freedom number i and zero for the other three degrees of freedom, gives four equations to determine $C_{i,j}$ for each i. In mathematical detail,

$$\begin{aligned}
\tilde{\varphi}_0(-1)=1, &\quad \tilde{\varphi}_0(1)=\tilde{\varphi}_0'(-1)=\tilde{\varphi}_i'(1)=0,\\
\tilde{\varphi}_1'(-1)=1, &\quad \tilde{\varphi}_1(-1)=\tilde{\varphi}_1(1)=\tilde{\varphi}_1'(1)=0,\\
\tilde{\varphi}_2(1)=1, &\quad \tilde{\varphi}_2(-1)=\tilde{\varphi}_2'(-1)=\tilde{\varphi}_2'(1)=0,\\
\tilde{\varphi}_3'(1)=1, &\quad \tilde{\varphi}_3(-1)=\tilde{\varphi}_3'(-1)=\tilde{\varphi}_3(1)=0\,.
\end{aligned}$$

These four 4×4 linear equations can be solved, yielding the following formulas for the cubic basis functions:

$$\tilde{\varphi}_0(X)=1-\frac{3}{4}(X+1)^2+\frac{1}{4}(X+1)^3 \tag{103}$$

$$\tilde{\varphi}_1(X)=-(X+1)(1-\frac{1}{2}(X+1))^2 \tag{104}$$

$$\tilde{\varphi}_2(X)=\frac{3}{4}(X+1)^2-\frac{1}{2}(X+1)^3 \tag{105}$$

$$\tilde{\varphi}_3(X)=-\frac{1}{2}(X+1)(\frac{1}{2}(X+1)^2-(X+1)) \tag{106}$$

$$\tag{107}$$

The construction of the dof map needs a scheme for numbering the global degrees of freedom. A natural left-to-right numbering has the function value at vertex x_i as degree of freedom number $2i$ and the value of the derivative at x_i as degree of freedom number $2i+1$, $i=0,\ldots,N_e+1$.

7 Numerical integration

Finite element codes usually apply numerical approximations to integrals. Since the integrands in the coefficient matrix often are (lower-order) polynomials, integration rules that can integrate polynomials exactly are popular.

The numerical integration rules can be expressed in a common form,

$$\int_{-1}^{1} g(X)\,\mathrm{d}X \approx \sum_{j=0}^{M} w_j g(\bar{X}_j), \tag{108}$$

where $\bar{X}_j$ are *integration points* and w_j are *integration weights*, $j = 0, \ldots, M$. Different rules correspond to different choices of points and weights.

The very simplest method is the *Midpoint rule*,

$$\int_{-1}^{1} g(X)\,\mathrm{d}X \approx 2g(0), \quad \bar{X}_0 = 0,\ w_0 = 2, \tag{109}$$

which integrates linear functions exactly.

7.1 Newton-Cotes rules

The Newton-Cotes rules are based on a fixed uniform distribution of the integration points. The first two formulas in this family are the well-known *Trapezoidal rule*,

$$\int_{-1}^{1} g(X)\,\mathrm{d}X \approx g(-1) + g(1), \quad \bar{X}_0 = -1,\ \bar{X}_1 = 1,\ w_0 = w_1 = 1, \tag{110}$$

and *Simpson's rule*,

$$\int_{-1}^{1} g(X)\,\mathrm{d}X \approx \frac{1}{3}\left(g(-1) + 4g(0) + g(1)\right), \tag{111}$$

where

$$\bar{X}_0 = -1,\ \bar{X}_1 = 0,\ \bar{X}_2 = 1,\ w_0 = w_2 = \frac{1}{3},\ w_1 = \frac{4}{3}\,. \tag{112}$$

Newton-Cotes rules up to five points is supported in the module file `numint.py`.

For higher accuracy one can divide the reference cell into a set of subintervals and use the rules above on each subinterval. This approach results in *composite* rules, well-known from basic introductions to numerical integration of $\int_a^b f(x)\,\mathrm{d}x$.

7.2 Gauss-Legendre rules with optimized points

More accurate rules, for a given M, arise if the location of the integration points are optimized for polynomial integrands. The Gauss-Legendre rules (also known as Gauss-Legendre quadrature or Gaussian quadrature) constitute one such class of integration methods. Two widely applied Gauss-Legendre rules in this family have the choice

$$M = 1: \quad \bar{X}_0 = -\frac{1}{\sqrt{3}},\ \bar{X}_1 = \frac{1}{\sqrt{3}},\ w_0 = w_1 = 1 \tag{113}$$

$$M = 2: \quad \bar{X}_0 = -\sqrt{\frac{3}{5}},\ \bar{X}_0 = 0,\ \bar{X}_2 = \sqrt{\frac{3}{5}},\ w_0 = w_2 = \frac{5}{9},\ w_1 = \frac{8}{9}\,. \tag{114}$$

These rules integrate 3rd and 5th degree polynomials exactly. In general, an M-point Gauss-Legendre rule integrates a polynomial of degree $2M+1$ exactly. The code `numint.py` contains a large collection of Gauss-Legendre rules.

8 Approximation of functions in 2D

All the concepts and algorithms developed for approximation of 1D functions $f(x)$ can readily be extended to 2D functions $f(x, y)$ and 3D functions $f(x, y, z)$. Basically, the extensions consist of defining basis functions $\psi_i(x, y)$ or $\psi_i(x, y, z)$ over some domain Ω, and for the least squares and Galerkin methods, the integration is done over Ω.

As in 1D, the least squares and projection/Galerkin methods lead to linear systems

$$\begin{aligned}
\sum_{j\in\mathcal{I}_s} A_{i,j}c_j &= b_i, \quad i \in \mathcal{I}_s,\\
A_{i,j} &= (\psi_i, \psi_j),\\
b_i &= (f, \psi_i),
\end{aligned}$$

where the inner product of two functions $f(x, y)$ and $g(x, y)$ is defined completely analogously to the 1D case (24):

$$(f, g) = \int_\Omega f(x, y)g(x, y)dxdy \tag{115}$$

8.1 2D basis functions as tensor products of 1D functions

One straightforward way to construct a basis in 2D is to combine 1D basis functions. Say we have the 1D vector space

$$V_x = \mathrm{span}\{\hat{\psi}_0(x), \ldots, \hat{\psi}_{N_x}(x)\}\,. \tag{116}$$

A similar space for a function's variation in y can be defined,

$$V_y = \mathrm{span}\{\hat{\psi}_0(y), \ldots, \hat{\psi}_{N_y}(y)\}\,. \tag{117}$$

We can then form 2D basis functions as *tensor products* of 1D basis functions.

Tensor products.

Given two vectors $a = (a_0, \ldots, a_M)$ and $b = (b_0, \ldots, b_N)$, their *outer tensor product*, also called the *dyadic product*, is $p = a \otimes b$, defined through

$$p_{i,j} = a_i b_j, \quad i = 0, \ldots, M,\ j = 0, \ldots, N\,.$$

In the tensor terminology, a and b are first-order tensors (vectors with one index, also termed rank-1 tensors), and then their outer tensor product is a second-order tensor (matrix with two indices, also termed rank-2 tensor). The corresponding *inner tensor product* is the well-known scalar or dot product of two vectors: $p = a \cdot b = \sum_{j=0}^{N} a_j b_j$. Now, p is a rank-0 tensor.

Tensors are typically represented by arrays in computer code. In the above example, a and b are represented by one-dimensional arrays of length M and N, respectively, while $p = a \otimes b$ must be represented by a two-dimensional array of size $M \times N$.

Tensor products can be used in a variety of context.

Given the vector spaces V_x and V_y as defined in (116) and (117), the tensor product space $V = V_x \otimes V_y$ has a basis formed as the tensor product of the basis for V_x and V_y. That is, if $\{\varphi_i(x)\}_{i\in\mathcal{I}_x}$ and $\{\varphi_i(y)\}_{i\in\mathcal{I}_y}$ are basis for V_x and V_y, respectively, the elements in the basis for V arise from the tensor product: $\{\varphi_i(x)\varphi_j(y)\}_{i\in\mathcal{I}_x, j\in\mathcal{I}_y}$. The index sets are $I_x = \{0, \ldots, N_x\}$ and $I_y = \{0, \ldots, N_y\}$.

The notation for a basis function in 2D can employ a double index as in

$$\psi_{p,q}(x, y) = \hat{\psi}_p(x)\hat{\psi}_q(y), \quad p \in \mathcal{I}_x, q \in \mathcal{I}_y\,.$$

The expansion for u is then written as a double sum

$$u = \sum_{p\in\mathcal{I}_x} \sum_{q\in\mathcal{I}_y} c_{p,q}\psi_{p,q}(x, y)\,.$$

Alternatively, we may employ a single index,

$$\psi_i(x, y) = \hat{\psi}_p(x)\hat{\psi}_q(y),$$

and use the standard form for u,

$$u = \sum_{j\in\mathcal{I}_s} c_j\psi_j(x, y)\,.$$

The single index is related to the double index through $i = p(N_y + 1) + q$ or $i = q(N_x + 1) + p$.

8.2 Example: Polynomial basis in 2D

Suppose we choose $\hat{\psi}_p(x) = x^p$, and try an approximation with $N_x = N_y = 1$:

$$\psi_{0,0} = 1, \quad \psi_{1,0} = x, \quad \psi_{0,1} = y, \quad \psi_{1,1} = xy\,.$$

Using a mapping to one index like $i = q(N_x + 1) + p$, we get

$$\psi_0 = 1, \quad \psi_1 = x, \quad \psi_2 = y, \quad \psi_3 = xy\,.$$

With the specific choice $f(x, y) = (1 + x^2)(1 + 2y^2)$ on $\Omega = [0, L_x] \times [0, L_y]$, we can perform actual calculations:

$$\begin{aligned}
A_{0,0} = (\psi_0, \psi_0) &= \int_0^{L_y}\int_0^{L_x} \psi_0(x, y)^2 dxdy = \int_0^{L_y}\int_0^{L_x} dxdy = L_x L_y, \\
A_{1,0} = (\psi_1, \psi_0) &= \int_0^{L_y}\int_0^{L_x} xdxdy = \frac{1}{2}L_x^2 L_y, \\
A_{0,1} = (\psi_0, \psi_1) &= \int_0^{L_y}\int_0^{L_x} ydxdy = \frac{1}{2}L_y^2 L_x, \\
A_{0,1} = (\psi_0, \psi_1) &= \int_0^{L_y}\int_0^{L_x} xydxdy = \int_0^{L_y} ydy \int_0^{L_x} xdx = \frac{1}{4}L_y^2 L_x^2\,.
\end{aligned}$$

The right-hand side vector has the entries

$$\begin{aligned}
b_0 = (\psi_0, f) &= \int_0^{L_y}\int_0^{L_x} 1 \cdot (1 + x^2)(1 + 2y^2)dxdy \\
&= \int_0^{L_y} (1 + 2y^2)dy \int_0^{L_x} (1 + x^2)dx = (L_y + \frac{2}{3}L_y^3)(L_x + \frac{1}{3}L_x^3) \\
b_1 = (\psi_1, f) &= \int_0^{L_y}\int_0^{L_x} x(1 + x^2)(1 + 2y^2)dxdy \\
&= \int_0^{L_y} (1 + 2y^2)dy \int_0^{L_x} x(1 + x^2)dx = (L_y + \frac{2}{3}L_y^3)(\frac{1}{2}L_x^2 + \frac{1}{4}L_x^4) \\
b_2 = (\psi_2, f) &= \int_0^{L_y}\int_0^{L_x} y(1 + x^2)(1 + 2y^2)dxdy \\
&= \int_0^{L_y} y(1 + 2y^2)dy \int_0^{L_x} (1 + x^2)dx = (\frac{1}{2}L_y + \frac{1}{2}L_y^4)(L_x + \frac{1}{3}L_x^3) \\
b_3 = (\psi_2, f) &= \int_0^{L_y}\int_0^{L_x} xy(1 + x^2)(1 + 2y^2)dxdy \\
&= \int_0^{L_y} y(1 + 2y^2)dy \int_0^{L_x} x(1 + x^2)dx = (\frac{1}{2}L_y^2 + \frac{1}{2}L_y^4)(\frac{1}{2}L_x^2 + \frac{1}{4}L_x^4)\,.
\end{aligned}$$

There is a general pattern in these calculations that we can explore. An arbitrary matrix entry has the formula

$$
\begin{aligned}
A_{i,j} &= (\psi_i, \psi_j) = \int_0^{L_y}\int_0^{L_x} \psi_i\psi_j dxdy \\
&= \int_0^{L_y}\int_0^{L_x} \psi_{p,q}\psi_{r,s} dxdy = \int_0^{L_y}\int_0^{L_x} \hat{\psi}_p(x)\hat{\psi}_q(y)\hat{\psi}_r(x)\hat{\psi}_s(y)dxdy \\
&= \int_0^{L_y} \hat{\psi}_q(y)\hat{\psi}_s(y)dy \int_0^{L_x} \hat{\psi}_p(x)\hat{\psi}_r(x)dx \\
&= \hat{A}^{(x)}_{p,r}\hat{A}^{(y)}_{q,s},
\end{aligned}
$$

where

$$
\hat{A}^{(x)}_{p,r} = \int_0^{L_x} \hat{\psi}_p(x)\hat{\psi}_r(x)dx, \quad \hat{A}^{(y)}_{q,s} = \int_0^{L_y} \hat{\psi}_q(y)\hat{\psi}_s(y)dy,
$$

are matrix entries for one-dimensional approximations. Moreover, $i = qN_y + q$ and $j = sN_y + r$.

With $\hat{\psi}_p(x) = x^p$ we have

$$
\hat{A}^{(x)}_{p,r} = \frac{1}{p+r+1}L_x^{p+r+1}, \quad \hat{A}^{(y)}_{q,s} = \frac{1}{q+s+1}L_y^{q+s+1},
$$

and

$$
A_{i,j} = \hat{A}^{(x)}_{p,r}\hat{A}^{(y)}_{q,s} = \frac{1}{p+r+1}L_x^{p+r+1}\frac{1}{q+s+1}L_y^{q+s+1},
$$

for $p, r \in \mathcal{I}_x$ and $q, s \in \mathcal{I}_y$.

Corresponding reasoning for the right-hand side leads to

$$
\begin{aligned}
b_i &= (\psi_i, f) = \int_0^{L_y}\int_0^{L_x} \psi_i f \, dxdx \\
&= \int_0^{L_y}\int_0^{L_x} \hat{\psi}_p(x)\hat{\psi}_q(y) f \, dxdx \\
&= \int_0^{L_y} \hat{\psi}_q(y)(1+2y^2)dy \int_0^{L_y} \hat{\psi}_p(x)x^p(1+x^2)dx \\
&= \int_0^{L_y} y^q(1+2y^2)dy \int_0^{L_y} x^p(1+x^2)dx \\
&= (\frac{1}{q+1}L_y^{q+1} + \frac{2}{q+3}L_y^{q+3})(\frac{1}{p+1}L_x^{p+1} + \frac{2}{q+3}L_x^{p+3})
\end{aligned}
$$

Choosing $L_x = L_y = 2$, we have

$$
A = \begin{bmatrix} 4 & 4 & 4 & 4 \\ 4 & \frac{16}{3} & 4 & \frac{16}{3} \\ 4 & 4 & \frac{16}{3} & \frac{16}{3} \\ 4 & \frac{16}{3} & \frac{16}{3} & \frac{64}{9} \end{bmatrix}, \quad b = \begin{bmatrix} \frac{308}{9} \\ \frac{140}{3} \\ 44 \\ 60 \end{bmatrix}, \quad c = \begin{bmatrix} -\frac{1}{9} \\ \frac{4}{3} \\ -\frac{2}{3} \\ 8 \end{bmatrix}.
$$

Figure 35 illustrates the result.

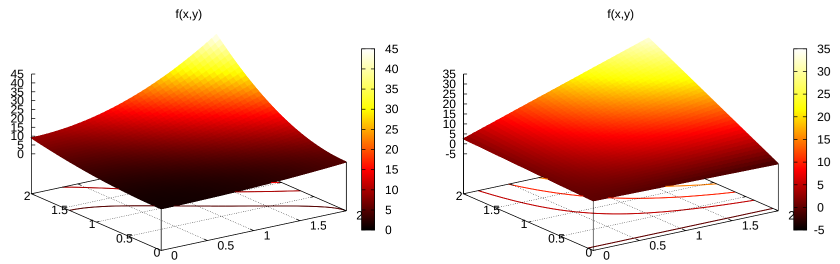


Figure 35: Approximation of a 2D quadratic function (left) by a 2D bilinear function (right) using the Galerkin or least squares method.

8.3 Implementation

The `least_squares` function from Section 2.8 and/or the file `approx1D.py` can with very small modifications solve 2D approximation problems. First, let `Omega` now be a list of the intervals in x and y direction. For example, $\Omega = [0, L_x] \times [0, L_y]$ can be represented by `Omega = [[0, L_x], [0, L_y]]`.

Second, the symbolic integration must be extended to 2D:

```
import sympy as sym

integrand = psi[i]*psi[j]
I = sym.integrate(integrand,
                  (x, Omega[0][0], Omega[0][1]),
                  (y, Omega[1][0], Omega[1][1]))
```

provided `integrand` is an expression involving the `sympy` symbols `x` and `y`. The 2D version of numerical integration becomes

```
if isinstance(I, sym.Integral):
    integrand = sym.lambdify([x,y], integrand)
    I = sym.mpmath.quad(integrand,
                        [Omega[0][0], Omega[0][1]],
                        [Omega[1][0], Omega[1][1]])
```

The right-hand side integrals are modified in a similar way.

Third, we must construct a list of 2D basis functions. Here are two examples based on tensor products of 1D "Taylor-style" polynomials x^i and 1D sine functions $\sin((i+1)\pi x)$:

```
def taylor(x, y, Nx, Ny):
    return [x**i*y**j for i in range(Nx+1) for j in range(Ny+1)]

def sines(x, y, Nx, Ny):
    return [sym.sin(sym.pi*(i+1)*x)*sym.sin(sym.pi*(j+1)*y)
            for i in range(Nx+1) for j in range(Ny+1)]
```

The complete code appears in `approx2D.py`.

The previous hand calculation where a quadratic f was approximated by a bilinear function can be computed symbolically by

```
>>> from approx2D import *
>>> f = (1+x**2)*(1+2*y**2)
>>> psi = taylor(x, y, 1, 1)
>>> Omega = [[0, 2], [0, 2]]
>>> u, c = least_squares(f, psi, Omega)
>>> print u
8*x*y - 2*x/3 + 4*y/3 - 1/9
>>> print sym.expand(f)
2*x**2*y**2 + x**2 + 2*y**2 + 1
```

We may continue with adding higher powers to the basis:

```
>>> psi = taylor(x, y, 2, 2)
>>> u, c = least_squares(f, psi, Omega)
>>> print u
2*x**2*y**2 + x**2 + 2*y**2 + 1
>>> print u-f
0
```

For $N_x \geq 2$ and $N_y \geq 2$ we recover the exact function f, as expected, since in that case $f \in V$ (see Section 2.5).

8.4 Extension to 3D

Extension to 3D is in principle straightforward once the 2D extension is understood. The only major difference is that we need the repeated outer tensor product,

$$V = V_x \otimes V_y \otimes V_z \,.$$

In general, given vectors (first-order tensors) $a^{(q)} = (a_0^{(q)}, \ldots, a_{N_q}^{(q)}$, $q = 0, \ldots, m$, the tensor product $p = a^{(0)} \otimes \cdots \otimes a^m$ has elements

$$p_{i_0,i_1,\ldots,i_m} = a_{i_1}^{(0)} a_{i_1}^{(1)} \cdots a_{i_m}^{(m)} \,.$$

The basis functions in 3D are then

$$\psi_{p,q,r}(x, y, z) = \hat{\psi}_p(x)\hat{\psi}_q(y)\hat{\psi}_r(z),$$

with $p \in \mathcal{I}_x$, $q \in \mathcal{I}_y$, $r \in \mathcal{I}_z$. The expansion of u becomes

$$u(x, y, z) = \sum_{p\in\mathcal{I}_x} \sum_{q\in\mathcal{I}_y} \sum_{r\in\mathcal{I}_z} c_{p,q,r}\psi_{p,q,r}(x, y, z) \,.$$

A single index can be introduced also here, e.g., $i = N_x N_y r + q_N x + p$, $u = \sum_i c_i \psi_i(x, y, z)$.

Use of tensor product spaces.

Constructing a multi-dimensional space and basis from tensor products of 1D spaces is a standard technique when working with global basis functions. In the world of finite elements, constructing basis functions by tensor products is much used on quadrilateral and hexahedra cell shapes, but not on triangles and tetrahedra. Also, the global finite element basis functions are almost exclusively denoted by a single index and not by the natural tuple of indices that arises from tensor products.

9 Finite elements in 2D and 3D

Finite element approximation is particularly powerful in 2D and 3D because the method can handle a geometrically complex domain Ω with ease. The principal idea is, as in 1D, to divide the domain into cells and use polynomials for approximating a function over a cell. Two popular cell shapes are triangles and quadrilaterals. Figures 36, 37, and 38 provide examples. P1 elements means linear functions ($a_0 + a_1x + a_2y$) over triangles, while Q1 elements have bilinear functions ($a_0 + a_1x + a_2y + a_3xy$) over rectangular cells. Higher-order elements can easily be defined.

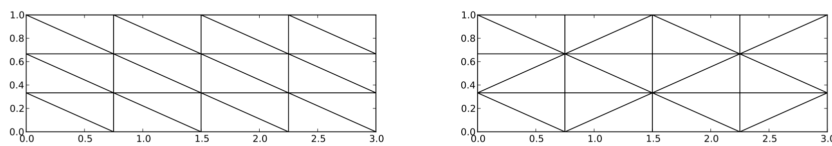


Figure 36: Examples on 2D P1 elements.

9.1 Basis functions over triangles in the physical domain

Cells with triangular shape will be in main focus here. With the P1 triangular element, u is a linear function over each cell, as depicted in Figure 39, with discontinuous derivatives at the cell boundaries.

We give the vertices of the cells global and local numbers as in 1D. The degrees of freedom in the P1 element are the function values at a set of nodes, which are the three vertices. The basis function $\varphi_i(x, y)$ is then 1 at the vertex with global vertex number i and zero at all other vertices. On an element, the three degrees of freedom uniquely determine the linear basis functions in that element, as usual. The global $\varphi_i(x, y)$ function is then a combination of the linear functions (planar surfaces) over all the neighboring cells that have vertex number i in common. Figure 40 tries to illustrate the shape of such a "pyramid"-like function.

Element matrices and vectors. As in 1D, we split the integral over Ω into a sum of integrals over cells. Also as in 1D, φ_i overlaps φ_j (i.e., $\varphi_i\varphi_j \neq 0$) if and only if i and j are vertices in the same cell. Therefore, the integral of $\varphi_i\varphi_j$ over an element is nonzero only when i and j run over the vertex numbers in the element. These nonzero contributions to the coefficient matrix are, as in 1D,

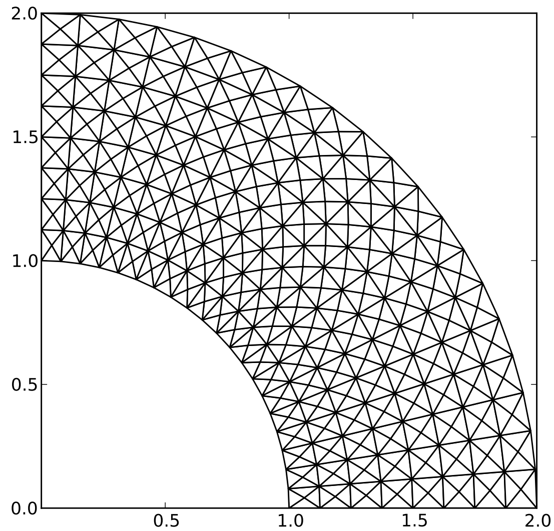


Figure 37: Examples on 2D P1 elements in a deformed geometry.

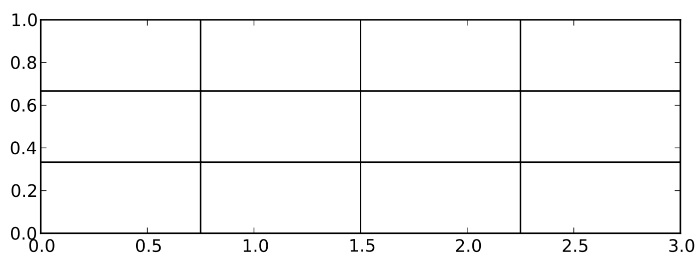


Figure 38: Examples on 2D Q1 elements.

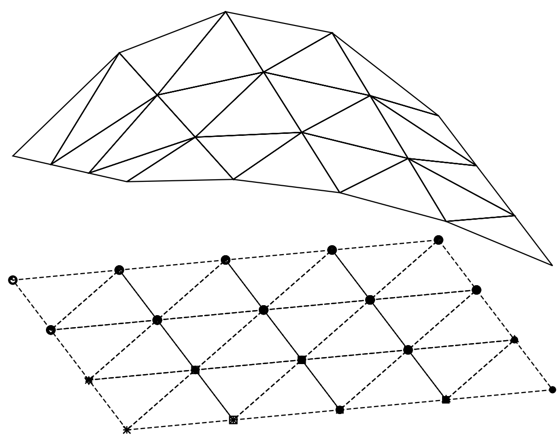


Figure 39: Example on piecewise linear 2D functions defined on triangles.

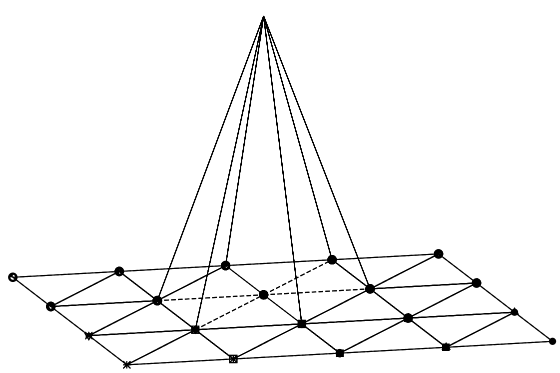


Figure 40: Example on a piecewise linear 2D basis function over a patch of triangles.

collected in an element matrix. The size of the element matrix becomes 3×3 since there are three degrees of freedom that i and j run over. Again, as in 1D, we number the local vertices in a cell, starting at 0, and add the entries in the element matrix into the global system matrix, exactly as in 1D. All details and code appear below.

9.2 Basis functions over triangles in the reference cell

As in 1D, we can define the basis functions and the degrees of freedom in a reference cell and then use a mapping from the reference coordinate system to the physical coordinate system. We also have a mapping of local degrees of freedom numbers to global degrees of freedom numbers.

The reference cell in an (X, Y) coordinate system has vertices $(0, 0)$, $(1, 0)$, and $(0, 1)$, corresponding to local vertex numbers 0, 1, and 2, respectively. The P1 element has linear functions $\tilde{\varphi}_r(X, Y)$ as basis functions, $r = 0, 1, 2$. Since a linear function $\tilde{\varphi}_r(X, Y)$ in 2D is on the form $C_{r,0} + C_{r,1}X + C_{r,2}Y$, and hence has three parameters $C_{r,0}$, $C_{r,1}$, and $C_{r,2}$, we need three degrees of freedom. These are in general taken as the function values at a set of nodes. For the P1 element the set of nodes is the three vertices. Figure 41 displays the geometry of the element and the location of the nodes.

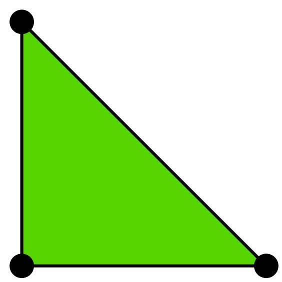


Figure 41: 2D P1 element.

Requiring $\tilde{\varphi}_r = 1$ at node number r and $\tilde{\varphi}_r = 0$ at the two other nodes, gives three linear equations to determine $C_{r,0}$, $C_{r,1}$, and $C_{r,2}$. The result is

$$\tilde{\varphi}_0(X, Y) = 1 - X - Y, \tag{118}$$
$$\tilde{\varphi}_1(X, Y) = X, \tag{119}$$
$$\tilde{\varphi}_2(X, Y) = Y \tag{120}$$

Higher-order approximations are obtained by increasing the polynomial order, adding additional nodes, and letting the degrees of freedom be function values at the nodes. Figure 42 shows the location of the six nodes in the P2 element.

A polynomial of degree p in X and Y has $n_p = (p + 1)(p + 2)/2$ terms and hence needs n_p nodes. The values at the nodes constitute n_p degrees of freedom. The location of the nodes for $\tilde{\varphi}_r$ up to degree 6 is displayed in Figure 43.

The generalization to 3D is straightforward: the reference element is a tetrahedron with vertices $(0, 0, 0)$, $(1, 0, 0)$, $(0, 1, 0)$, and $(0, 0, 1)$ in a X, Y, Z

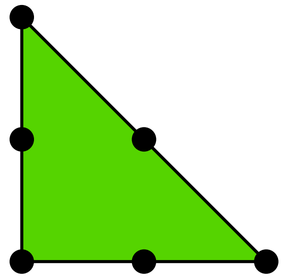


Figure 42: 2D P2 element.

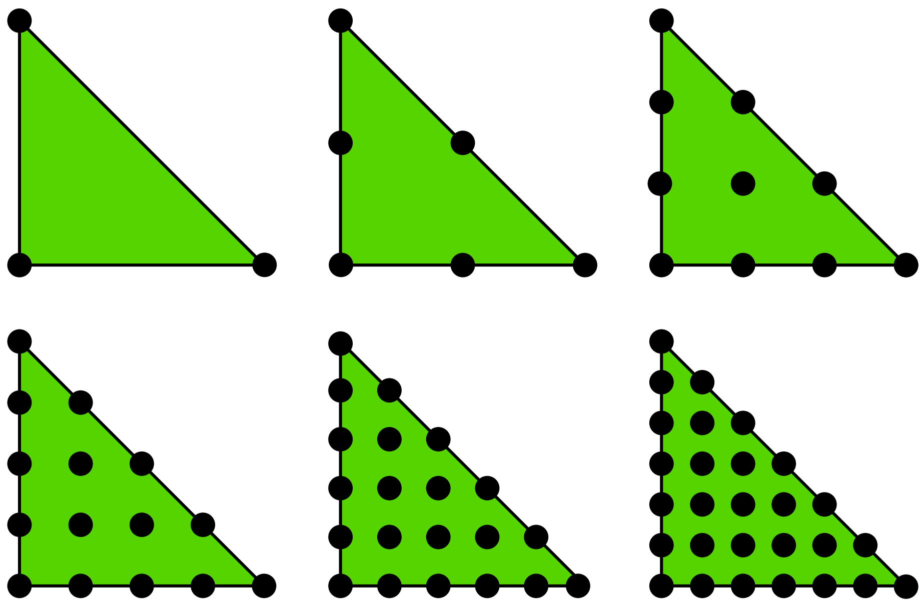


Figure 43: 2D P1, P2, P3, P4, P5, and P6 elements.

reference coordinate system. The P1 element has its degrees of freedom as four nodes, which are the four vertices, see Figure 44. The P2 element adds additional nodes along the edges of the cell, yielding a total of 10 nodes and degrees of freedom, see Figure 45.

The interval in 1D, the triangle in 2D, the tetrahedron in 3D, and its generalizations to higher space dimensions are known as *simplex* cells (the geometry) or *simplex* elements (the geometry, basis functions, degrees of freedom, etc.). The plural forms simplices and simplexes are also a much used shorter terms when referring to this type of cells or elements. The side of a simplex is called a *face*, while the tetrahedron also has *edges*.

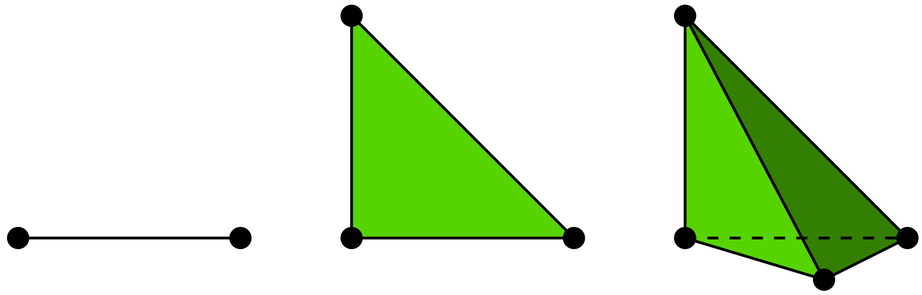


Figure 44: P1 elements in 1D, 2D, and 3D.

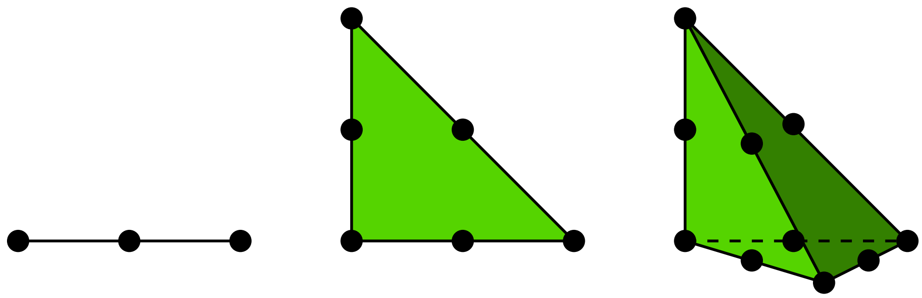


Figure 45: P2 elements in 1D, 2D, and 3D.

Acknowledgment. Figures 41-45 are created by Anders Logg and taken from the FEniCS book: *Automated Solution of Differential Equations by the Finite Element Method*, edited by A. Logg, K.-A. Mardal, and G. N. Wells, published by Springer, 2012.

9.3 Affine mapping of the reference cell

Let $\tilde{\varphi}_r^{(1)}$ denote the basis functions associated with the P1 element in 1D, 2D, or 3D, and let $\boldsymbol{x}_{q(e,r)}$ be the physical coordinates of local vertex number r in cell e. Furthermore, let $\boldsymbol{X}$ be a point in the reference coordinate system corresponding to the point $\boldsymbol{x}$ in the physical coordinate system. The affine mapping of any $\boldsymbol{X}$ onto $\boldsymbol{x}$ is then defined by

$$\boldsymbol{x} = \sum_r \tilde{\varphi}_r^{(1)}(\boldsymbol{X})\boldsymbol{x}_{q(e,r)}, \tag{121}$$

where r runs over the local vertex numbers in the cell. The affine mapping essentially stretches, translates, and rotates the triangle. Straight or planar faces of the reference cell are therefore mapped onto straight or planar faces in the physical coordinate system. The mapping can be used for both P1 and higher-order elements, but note that the mapping itself always applies the P1 basis functions.

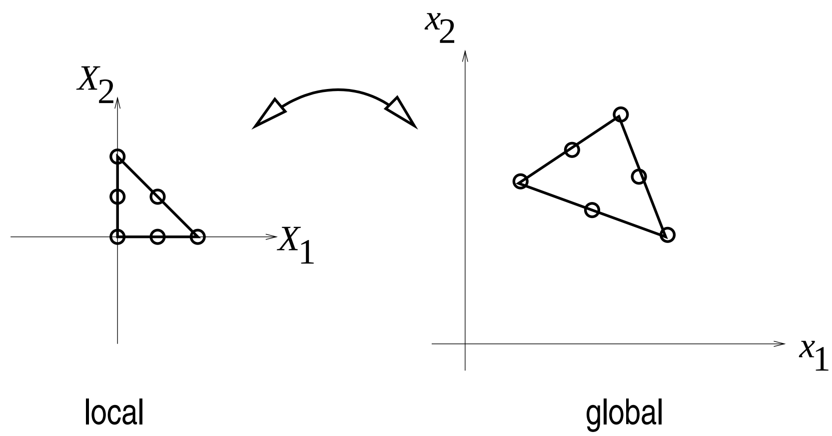


Figure 46: Affine mapping of a P1 element.

9.4 Isoparametric mapping of the reference cell

Instead of using the P1 basis functions in the mapping (121), we may use the basis functions of the actual Pd element:

$$\boldsymbol{x} = \sum_r \tilde{\varphi}_r(\boldsymbol{X})\boldsymbol{x}_{q(e,r)}, \tag{122}$$

where r runs over all nodes, i.e., all points associated with the degrees of freedom. This is called an *isoparametric mapping*. For P1 elements it is identical to the affine mapping (121), but for higher-order elements the mapping of the straight or planar faces of the reference cell will result in a *curved* face in the physical coordinate system. For example, when we use the basis functions of the triangular P2 element in 2D in (122), the straight faces of the reference triangle are mapped onto curved faces of parabolic shape in the physical coordinate system, see Figure 47.

From (121) or (122) it is easy to realize that the vertices are correctly mapped. Consider a vertex with local number s. Then $\tilde{\varphi}_s = 1$ at this vertex and zero at the others. This means that only one term in the sum is nonzero and $\boldsymbol{x} = \boldsymbol{x}_{q(e,s)}$, which is the coordinate of this vertex in the global coordinate system.

9.5 Computing integrals

Let $\tilde{\Omega}^r$ denote the reference cell and $\Omega^{(e)}$ the cell in the physical coordinate system. The transformation of the integral from the physical to the reference coordinate system reads

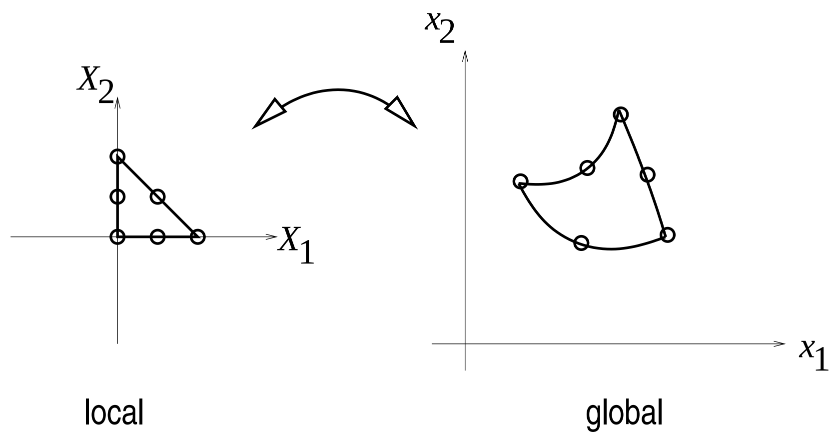


Figure 47: Isoparametric mapping of a P2 element.

$$\int_{\Omega^{(e)}} \varphi_i(\boldsymbol{x})\varphi_j(\boldsymbol{x})\,\mathrm{d}x = \int_{\tilde{\Omega}^r} \tilde{\varphi}_i(\boldsymbol{X})\tilde{\varphi}_j(\boldsymbol{X}) \det J\ \mathrm{d}X, \tag{123}$$

$$\int_{\Omega^{(e)}} \varphi_i(\boldsymbol{x})f(\boldsymbol{x})\,\mathrm{d}x = \int_{\tilde{\Omega}^r} \tilde{\varphi}_i(\boldsymbol{X})f(\boldsymbol{x}(\boldsymbol{X})) \det J\ \mathrm{d}X, \tag{124}$$

where $\mathrm{d}x$ means the infinitesimal area element $dxdy$ in 2D and $dxdydz$ in 3D, with a similar definition of $\mathrm{d}X$. The quantity $\det J$ is the determinant of the Jacobian of the mapping $\boldsymbol{x}(\boldsymbol{X})$. In 2D,

$$J = \left[\begin{array}{cc} \frac{\partial x}{\partial X} & \frac{\partial x}{\partial Y} \\ \frac{\partial y}{\partial X} & \frac{\partial y}{\partial Y} \end{array}\right], \quad \det J = \frac{\partial x}{\partial X}\frac{\partial y}{\partial Y} - \frac{\partial x}{\partial Y}\frac{\partial y}{\partial X}\,. \tag{125}$$

With the affine mapping (121), $\det J = 2\Delta$, where Δ is the area or volume of the cell in the physical coordinate system.

Remark. Observe that finite elements in 2D and 3D builds on the same *ideas* and *concepts* as in 1D, but there is simply much more to compute because the specific mathematical formulas in 2D and 3D are more complicated and the book keeping with dof maps also gets more complicated. The manual work is tedious, lengthy, and error-prone so automation by the computer is a must.

10 Exercises

Problem 1: Linear algebra refresher

Look up the topic of *vector space* in your favorite linear algebra book or search for the term at Wikipedia.

a) Prove that vectors in the plane (a, b) form a vector space by showing that all the axioms of a vector space are satisfied.

Solution. The axioms of a vector space go as follows (see Wikipedia, but we use slightly different notation below):

1. The sum of u and v, denoted by $u + v$, is in V.
2. $u + v = v + u$.
3. $(u + v) + w = u + (v + w)$.
4. There is a *zero* vector 0 in V such that $u + 0 = u$.
5. For each u in V, there is a vector $-u$ in V such that $u + (-u) = 0$.
6. The scalar multiple of u by γ, denoted by γu, is in V.
7. $\gamma(u + v) = \gamma u + \gamma v$.
8. $(\gamma + \delta)u = \gamma u + \delta u$ for scalar γ and δ.
9. $\gamma(\delta u) = \gamma\delta u$.
10. $1u = u$.

We must show that each axiom is fulfilled by planar vectors and their mathematical rules. Let $u = (a, b)$ and $v = (c, d)$.

Axiom 1:

$$u + v = (a, b) + (c, d) = (a + c, b + d),$$

is a planar vector and therefore in V.

Axiom 2:

$$u + v = (a, b) + (c, d) = (a + c, b + d) = (c + a, d + b) = v + u\,.$$

Axiom 3:

$$(u + v) + w = ((a, b) + (c, d)) + (e, f) = (a, b) + ((c, d) + (e, f)) = u + (v + w)\,.$$

Axiom 4: The $(0, 0)$ vector is the 0 element,

$$u + 0 = (a, b) + (0, 0) = (a + 0, b + 0) = (a, b) = u\,.$$

Axiom 5: Let $-u$ element is $(-a, -b)$, so

$$u + (-u) = (a, b) + (-a, -b) = (0, 0) = 0\,.$$

Axiom 6:

$$\gamma u = \gamma \cdot (a, b) = (\gamma a, \gamma b),$$

is also a planar vector and therefore in V.

Axiom 7:

$$\gamma(u + v) = \gamma \cdot ((a, b) + (c, d) = \gamma(a, b) + \gamma(c, d)\,.$$

Axiom 8:

$$(\gamma + \delta)u = (\gamma + \delta)(a, b) = \gamma(a, b) + \delta(a, b) = \gamma u + \delta u\,.$$

Axiom 9:

$$\gamma(\delta u) = \gamma(\delta \cdot (a, b)) = \gamma(\delta a, \delta b) = (\gamma\delta a, \gamma\delta b) = \gamma\delta u\,.$$

Axiom 10:

$$1u = 1(a, b) = (1 \cdot a, 1 \cdot b) = (a, b) = u\,.$$

b) Prove that all linear functions of the form $ax + b$ constitute a vector space, $a, b \in \mathbb{R}$.

Solution. Let $u = ax + b$ and $v = cx + d$. We verify each axiom.

Axiom 1:

$$u + v = ax + b + cx + d = (a + c)x + (b + d),$$

is also a linear function and therefore in V.

Axiom 2:

$$u + v = ax + b + cx + d = cx + d + ax + b = v + u\,.$$

Axiom 3:

$$(u+v)+w = (ax+b+cx+d)+ex+f = ax+b+cx+d+ex+fax+b+(cx+d+ex+f) = u+(v+w)\,.$$

Axiom 4: The $0x + 0 = 0$ function is the 0 element,

$$u + 0 = ax + b + 0 = ax + b = u\,.$$

Axiom 5: Let $-u$ element is $-ax - b$, so

$$u + (-u) = ax + b + (-ax - b) = 0\,.$$

Axiom 6:

$$\gamma u = \gamma(ax + b) = \gamma ax + \gamma b,$$

is also a linear function and therefore in V.

Axiom 7:

$$\gamma(u+v) = \gamma(ax+b+cx+d) = \gamma ax+\gamma b+\gamma cx+\gamma d = \gamma(ax+b)+\gamma(cd+d) = \gamma u+\gamma v\,.$$

Axiom 8:

$$(\gamma + \delta)u = (\gamma + \delta)(ax + b) = \gamma(ax + b) + \delta(ax + b) = \gamma u + \delta u\,.$$

Axiom 9:

$$\gamma(\delta u) = \gamma(\delta(ax + b))) = \gamma\delta u\,.$$

Axiom 10:

$$1u = 1(ax + b) = ax + b = u\,.$$

c) Show that all quadratic functions of the form $1 + ax^2 + bx$ *do not* constitute a vector space.

Solution. Let $u = ax^2 + bx + 1$ and $v = cx^2 + dx + 1$. We try to verify each axiom.

Axiom 1:

$$u + v = ax^2 + bx + 1 + cx^2 + dx + 1 = (a + c)x^2 + (b + d)x + 2,$$

but this quadratic function is not in V because the constant term is 2 and not 1. Consequently, quadratic functions of the particular form $1 + ax^2 + bx$ do not constitute a vector space. The more general form $ax^2 + bx + c$ for arbitrary constants a, b, and c makes functions that span a function space.

d) Check out the topic of *inner product spaces*. Suggest a possible inner product for the space of all linear functions of the form $ax + b$, $a, b \in \mathbb{R}$, defined on some interval $\Omega = [A, B]$. Show that this particular inner product satisfies the general requirements of an inner product in a vector space.

Solution. According to Wikipedia, an inner product space, with an inner product (u, v), has three axioms (we drop the possibility of complex numbers and assume everything is real):

1. Symmetry: $(u, v) = (v, u)$
2. Linearity in the first argument: $\gamma u, v) = \gamma(u, v)$
3. Positive-definiteness: $(u, u) \geq 0$ and $(u, u) = 0$ implies $u = 0$

A possible inner product for linear functions on a domain Ω is

$$(u, v) = \int_A^B uv \,\mathrm{d}x = \int_A^B (ax + b)(cx + d) \,\mathrm{d}x \,.$$

Symmetry is obvious since $uv = vu$:

$$(u, v) = \int_A^B uv \,\mathrm{d}x = \int_A^B vud = (v, u) \,.$$

Linearity in the first argument:

$$(\gamma u, v) = \gamma \int_A^B (\gamma u)v \,\mathrm{d}x = \gamma \int_A^B uv \,\mathrm{d}x = \gamma(u, v) \,.$$

Positive-definiteness:

$$(u, u) = \int_A^B (ax + b)^2 \,\mathrm{d}x \geq 0,$$

since the integral of a function $f(x) \geq$ must be greater than or equal to zero, and in particular,

$$(u, u) = 0 \quad \Rightarrow \quad \int_A^B (ax + b)^2 \,\mathrm{d}x = 0,$$

implies $ax + b = 0$.
Filename: `linalg1`.

Problem 2: Approximate a three-dimensional vector in a plane

Given $\boldsymbol{f} = (1, 1, 1)$ in $\mathbb{R}^3$, find the best approximation vector $\boldsymbol{u}$ in the plane spanned by the unit vectors $(1, 0)$ and $(0, 1)$. Repeat the calculations using the vectors $(2, 1)$ and $(1, 2)$.

Solution. We have the vector $\boldsymbol{f} = (1, 1, 1)$. Our aim is to approximate this with a vector in the vector-space spanned by the unit vectors $\boldsymbol{\phi_0}$ and $\boldsymbol{\phi_1}$. We seek a solution $u = c_0\phi_0 + c_1\phi_1$. To do this we use the least-square-method and solve the equation $\boldsymbol{Ac} = \boldsymbol{b}$. Or written out:

$$\begin{bmatrix} A_{0,0} & A_{0,1} \\ A_{1,0} & A_{1,1} \end{bmatrix} \begin{bmatrix} c_0 \\ c_1 \end{bmatrix} = \begin{bmatrix} b_0 \\ b_1 \end{bmatrix}$$

where $A_{i,j} = (\boldsymbol{\phi_i}, \boldsymbol{\phi_j})$ and $b_i = (\boldsymbol{\phi_i}, \boldsymbol{f})$.

We start with $\boldsymbol{\phi_0} = (0, 1)$, $\boldsymbol{\phi_1} = (1, 0)$. Calculations give

$$A_{0,0} = ([1, 0], [1, 0]) = 1,$$
$$A_{0,1} = ([1, 0], [0, 1]) = 0, A_{1,0} \quad = ([0, 1], [1, 0]) = 0, A_{1,1} = ([0, 1], [0, 1]) = 1, b_0 \quad = ([1, 0], [1, 1, 1]) = 1, b_0 = ([0,$$

The result becomes $c_0 = c_1 = 1$, and hence

$$u = 1 \cdot \boldsymbol{\phi_0} + 1 \cdot \boldsymbol{\phi_1}.$$

Then we proceed with $\boldsymbol{\phi_0} = (2,1)$, $\boldsymbol{\phi_1} = (1,2)$. Calculations give

$$A_{0,0} = ([2,1],[2,1]) = 2 \cdot 2 + 1 \cdot 1 = 5, A_{0,1} \quad = ([2,1],[1,2]) = 2 \cdot 1 + 1 \cdot 2 = 4, A_{1,0} = ([1,2],[2,1]) = 1 \cdot 2 + 2 \cdot$$

Solving for the c_i values results in $c_0 = c_1 = \frac{1}{3}$ and hence

$$u = \frac{1}{3} \cdot \boldsymbol{\phi_0} + \frac{1}{3} \cdot \boldsymbol{\phi_1}.$$

Filename: `vec111_approx`.

Problem 3: Approximate a parabola by a sine

Given the function $f(x) = 1 + 2x(1-x)$ on $\Omega = [0,1]$, we want to find an approximation in the function space

$$V = \text{span}\{1, \sin(\pi x)\}\,.$$

a) Sketch or plot $f(x)$. Think intuitively how an expansion in terms of the basis functions of V, $\psi_0(x) = 1$, $\psi_1(x) = \sin(\pi x)$, can be construction to yield a best approximation to f. Or phrased differently, see if you can guess the coefficients c_0 and c_1 in the expansion

$$u(x) = c_0\psi_0 + c_1\psi_1 = c_0 + c_1 \sin(\pi x)\,.$$

Compute the L^2 error $||f-u||_{L^2} = (\int_0^1 (f-u)^2\,\mathrm{d}x)^{1/2}$.

Hint. If you make a mesh function `e` of the error on some mesh with uniformly spaced coordinates in the array `xc`, the integral can be approximated as `np.sqrt(dx*np.sum(e**2))`, where `dx=xc[0]-xc[1]` is the mesh spacing and `np` is an alias for the `numpy` module in Python.

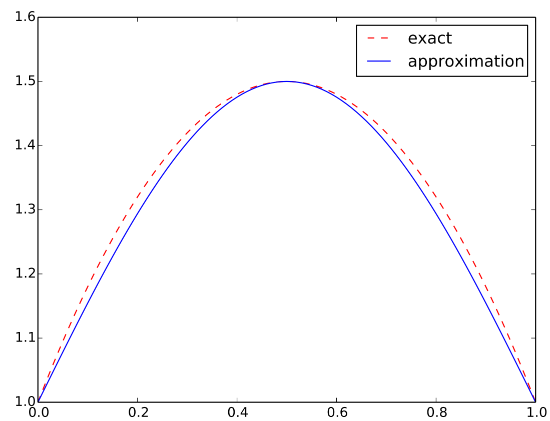
Solution. The function $\psi_0 = 1$ can be used to "take care of" of the constant 1 in f, while $\psi_1 = \sin(\pi x)$ can approximate the parabola. The maximum of f is $3/2$, so we should use $u(x) = 1 \cdot \psi_0 + \frac{1}{2}\psi_1$.

Plotting and the computation of the L^2 error can be done by

```
import numpy as np
import matplotlib.pyplot as plt

xc = np.linspace(0, 1, 101)  # x coordinates for plotting

def f(x):
    return 1 + 2*x*(1-x)

import sympy as sym
```

```
x = sym.symbols('x')
psi_0 = 1
psi_1 = sym.sin(sym.pi*x)

half = sym.Rational(1,2)
u = 1*psi_0 + half*psi_1

# How to combine c_0*psi_0 + c_1*psi_1 to match f?
# Intuitively, c_0=c_1=1...
# Turn u to function so we can plot and compute with it
u = sym.lambdify([x], u, modules='numpy')

print 'L2 error of intuitive approximation:',
e = f(xc) - u(xc)
dx = xc[1] - xc[0]
print np.sqrt(dx*np.sum(e**2))

plt.plot(xc, f(xc), 'r--')
plt.plot(xc, u(xc), 'b-')
plt.legend(['exact', 'intuitive approximation'])
```

The L^2 error becomes 0.0179.



b) Perform the hand calculations for a least squares approximation.

Solution. The least squares method ends up with a linear system where the coefficient matrix has entries $A_{i,j} = \int_0^1 \psi_i \psi_j \, dx$ and the right-hand side has entries $b_i = \int_0^1 \psi_i \, dx$. We can use `sympy` do carry out the integrals:

```
# Do the calculations in the least squares or project method
A = sym.zeros((2, 2))
b = sym.zeros((2, 1))
A[0,0] = sym.integrate(psi_0*psi_0, (x, 0, 1))
A[0,1] = sym.integrate(psi_0*psi_1, (x, 0, 1))
A[1,0] = A[0,1]
A[1,1] = sym.integrate(psi_1*psi_1, (x, 0, 1))
b[0] = sym.integrate(f(x)*psi_0, (x, 0, 1))
b[1] = sym.integrate(f(x)*psi_1, (x, 0, 1))
print 'A:', A
```

```
print 'b:', b
c = A.LUsolve(b)
c = [sym.simplify(c[i,0]) for i in range(c.shape[0])]
print 'c:', c, [c_.evalf() for c_ in c]
u = c[0]*psi_0 + c[1]*psi_1
print 'u:', u
```

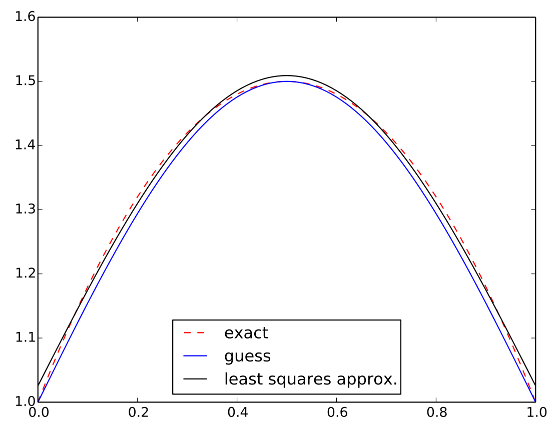
Looking at the results, we get the linear system

$$\begin{pmatrix} 1 & \frac{2}{\pi} \\ \frac{2}{\pi} & \frac{1}{2} \end{pmatrix} \left(\begin{bmatrix} \frac{-24\pi^2-96+4\pi^4}{3\pi^2(-8+\pi^2)} \\ \frac{-4\pi^2+48}{3\pi(-8+\pi^2)} \end{bmatrix} \right) = \begin{pmatrix} \frac{4}{3} \\ \frac{8}{\pi^3} + \frac{2}{\pi} \end{pmatrix}$$

The resulting best approximation reads

$$u(x) = \frac{4\left(-\pi^2+12\right)\sin\left(\pi x\right)}{3\pi\left(-8+\pi^2\right)} + \frac{-24\pi^2-96+4\pi^4}{3\pi^2\left(-8+\pi^2\right)} \approx 1.025 + 0.484\sin(\pi x)$$

The L^2 error turns out to be 0.00876. To conclude, the least squares method is slightly better than the intuition in this case.



Filename: `parabola_sin`.

Problem 4: Approximate the exponential function by power functions

Let V be a function space with basis functions x^i, $i = 0, 1, \ldots, N$. Find the best approximation to $f(x) = \exp(-x)$ on $\Omega = [0, 8]$ among all functions in V for $N = 2, 4, 6$. Illustrate the three approximations in three separate plots.

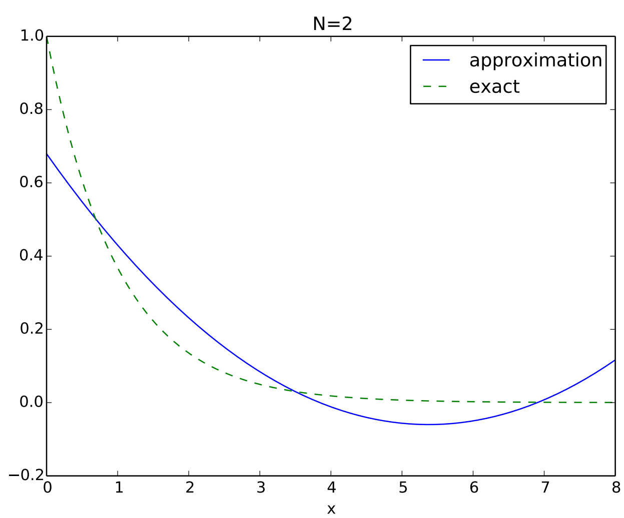
Hint. Apply the `lest_squares` and `comparison_plot` functions in the `approx1D.py` module as these make the exercise easier to solve.

Solution. A suitable code is

```
from approx1D import least_squares, comparison_plot
import matplotlib.pyplot as plt
import sympy as sym
from math import factorial
import numpy as np

x = sym.Symbol('x')
f = sym.exp(-x)

Omega = [0, 8]

for N in 2,4,6:
    psi = [x**i for i in range(N+1)]
    u, c = least_squares(f,psi,Omega)
    print N, u
    plt.figure()
    comparison_plot(f, u, Omega, filename='tmp_exp_%d' % N,
                    plot_title='N=%d' % N)
```

For the case $N = 2$ the program prints the following, here edited for clearer reading:

```
A:
Matrix([[8, 32, 512/3], [32, 512/3, 1024], [512/3, 1024, 32768/5]])
b:
Matrix([[-exp(-8) + 1], [-9*exp(-8) + 1], [-82*exp(-8) + 2]])

f: exp(-x)
u: x**2*(-465*exp(-8)/4096 + 105/4096) + x*(-141/512 +
   405*exp(-8)/512) - 111*exp(-8)/128 + 87/128
```



Filename: `exp_powers`.

Problem 5: Approximate the sine function by power functions

In this exercise we want to approximate the sine function by polynomials of order $N+1$. Consider two bases:

$$V_1 = \{x, x^3, x^5, \ldots, x^{N-2}, x^N\},$$
$$V_2 = \{1, x, x^2, x^3, \ldots, x^N\}.$$

The basis V_1 is motivated by the fact that the Taylor polynomial approximation to the sine function has only odd powers, while V_2 is motivated by the assumption that also the even powers could improve the approximation in a least-squares setting.

Compute the best approximation to $f(x) = \sin(x)$ among all functions in V_1 and V_2 on two domains of increasing sizes: $\Omega_{1,k} = [0, k\pi]$, $k = 2, 3 \ldots, 6$ and $\Omega_{2,k} = [-k\pi/2, k\pi/2]$, $k = 2, 3, 4, 5$. Make plots for all combinations of V_1, V_2, Ω_1, Ω_2, $k = 2, 3, \ldots, 6$.

Add a plot of the N-th degree Taylor polynomial approximation of $\sin(x)$ around $x = 0$.

Hint. You can make a loop over V_1 and V_2, a loop over Ω_1 and Ω_2, and a loop over k. Inside the loops, call the functions `least_squares` and `comparison_plot` from the `approx1D` module. $N = 7$ is a suggested value.

Solution. Suitable code is

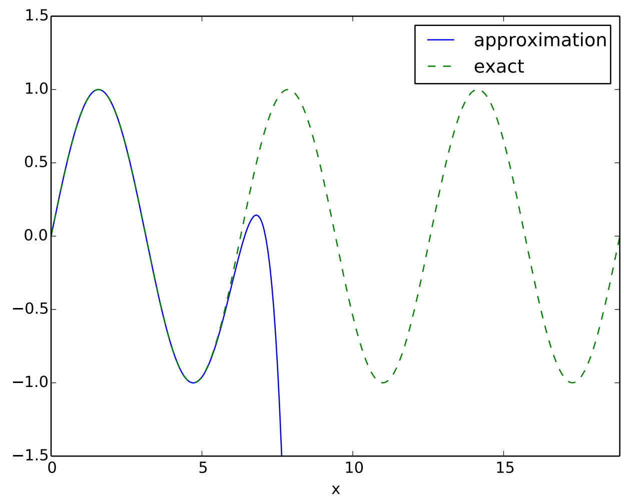
```
import sympy as sym
from approx1D import least_squares, comparison_plot
from math import pi
import matplotlib.pyplot as plt

x = sym.Symbol('x')
f = sym.sin(x)
N = 7
psi_bases = [[x**i for i in range(1, N+1, 2)],  # V_1
             [x**i for i in range(0, N+1)]]     # V_2
symbolic = False

for V, psi in enumerate(psi_bases):
    for domain_no in range(1, 3):
        for k in range(2, 6):
            if symbolic:
                Omega = [0, k*sym.pi] if domain_no == 1 else \
                        [-k*sym.pi/2, k*sym.pi/2]
            else:
                # cannot use sym.pi with numerical sympy computing
                Omega = [0, k*pi] if domain_no == 1 else \
                        [-k*pi/2, k*pi/2]

            u, c = least_squares(f, psi, Omega, symbolic=symbolic)

            comparison_plot(
```

```
                f, u, Omega,
                ymin=-2, ymax=2,
                filename='tmp_N%d_V%dOmega%dk%d' %
                (N, V, k, domain_no),
                plot_title='sin(x) on [0,%d*pi/2] by %s' %
                (k, ','.join([str(p) for p in psi])))
            # Need to kill the plot to proceed!
        for ext in 'png', 'pdf':
            cmd = 'doconce combine_images -2 ' + \
                  ' '.join(['tmp_N%d_V%dOmega%dk%d.' %
                            (N, V, k, domain_no) + ext
                            for k in range(2, 6)]) + \
                  ' sin_powers_N%d_V%d_Omega%d.' % (N, V, domain_no) + ext
            print cmd
            os.system(cmd)

# Show the standard Taylor series approximation
from math import factorial, pi
import time
Omega = [0, 12*pi/2.]
u = 0
for k in range(0,N+1):
    u = u + ((-1)**k*x**(1+2*k))/float(factorial(1+2*k))
# Shorter: u = sum(((-1)**k*x**(1+2*k))/float(factorial(1+2*k))
# for k in range(0,10))
comparison_plot(f, u, Omega, 'sin_taylor%d' % k,
                ymin=-1.5, ymax=1.5)
```

The odd powers (V_1 space) behave not so good on $\Omega_{1,k}$, but better on $\Omega_{2,k}$:

Including also even powers (V_2 space) is clearly much better:

Comparison with a standard Taylor series shows that it is very inferior as an approximation over the entire domain, but much more accurate close to the origin (as expected, since the Taylor series is constructed with this property, while the least squares method tries to find a good approximation over the entire domain).



Filename: `sin_powers`.

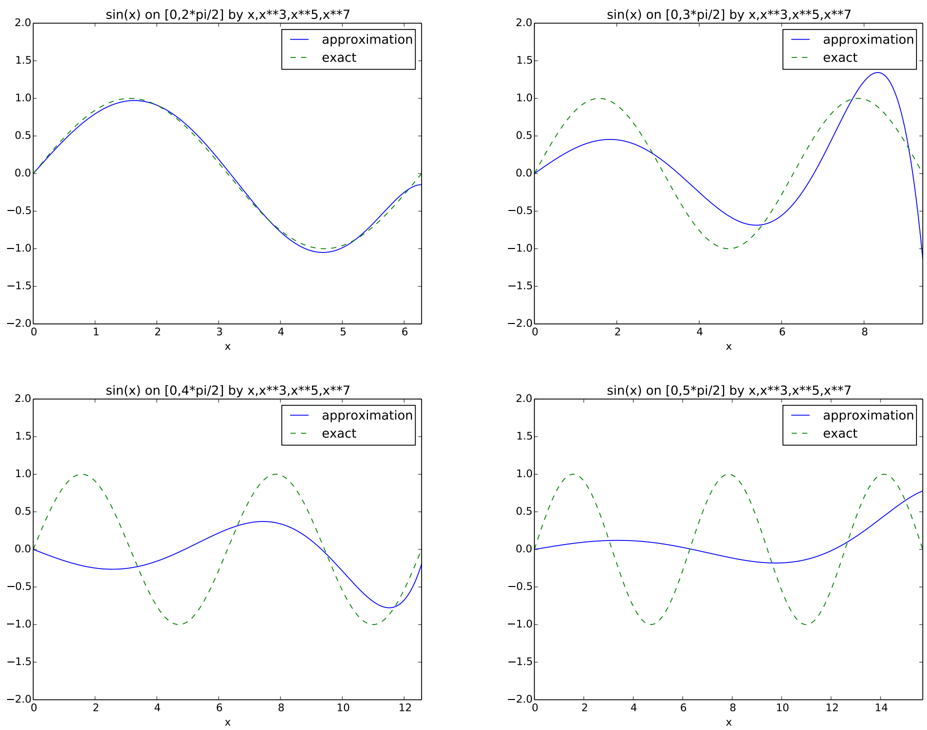


Figure 48: V_1 space, $\Omega_{1,k}$ domain.

Problem 6: Approximate a steep function by sines

Find the best approximation of $f(x) = \tanh(s(x - \pi))$ on $[0, 2\pi]$ in the space V with basis $\psi_i(x) = \sin((2i + 1)x)$, $i \in \mathcal{I}_s = \{0, \ldots, N\}$. Make a movie showing how $u = \sum_{j\in\mathcal{I}_s} c_j\psi_j(x)$ approximates $f(x)$ as N grows. Choose s such that f is steep ($s = 20$ is appropriate).

Hint 1. One may naively call the `least_squares_orth` and `comparison_plot` from the `approx1D` module in a loop and extend the basis with one new element in each pass. This approach implies a lot of recomputations. A more efficient strategy is to let `least_squares_orth` compute with only one basis function at a time and accumulate the corresponding `u` in the total solution.

Hint 2. `ffmpeg` or `avconv` may skip frames when plot files are combined to a movie. Since there are few files and we want to see each of them, use `convert` to make an animated GIF file (`-delay 200` is suitable).

Solution. The code may read

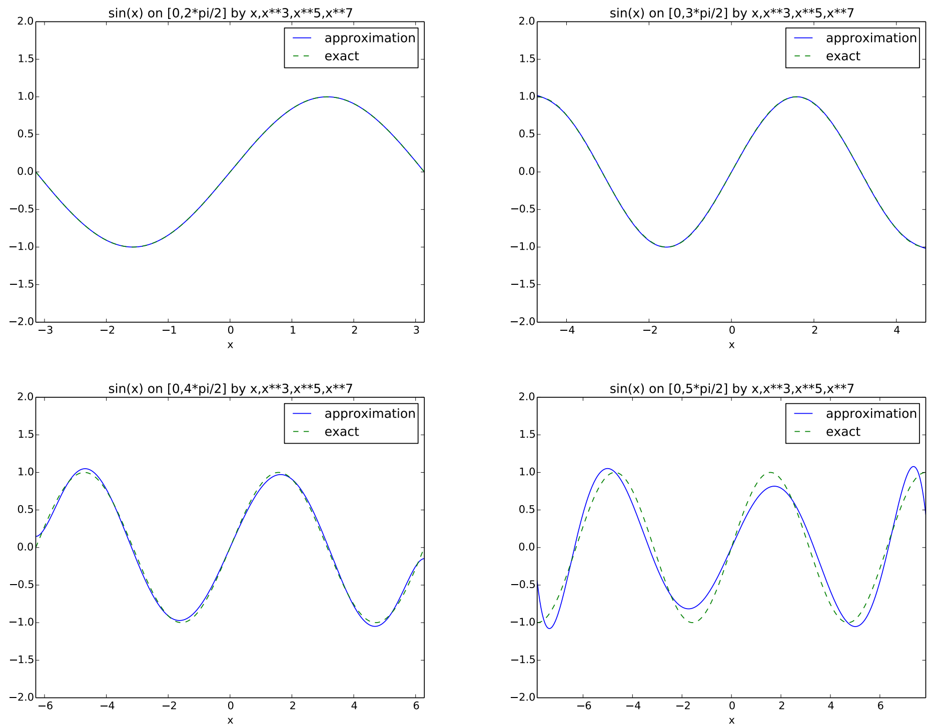


Figure 49: V_1 space, $\Omega_{2,k}$ domain.

```
import sympy as sym
from approx1D import least_squares_orth, comparison_plot
import matplotlib.pyplot as plt

x = sym.Symbol('x')

# Naive approach: (not utilizing the fact that i+1 computations can
# make use of i computations)
def naive(f, s, Omega, N=10):
    psi = []
    for i in range(N+1):
        psi.append(sym.sin((2*i+1)*x))
        u, c = least_squares_orth(f, psi, Omega, symbolic=False)
        comparison_plot(f, u, Omega, 'tmp_sin%02dx' % i,
                        legend_loc='upper left', show=True)

# Efficient approach: compute just the matrix diagonal
def efficient(f, s, Omega, N=10):
    u = 0
    for i in range(N+1):
        psi = [sym.sin((2*i+1)*x)]
        next_term, c = least_squares_orth(f, psi, Omega, False)
        u = u + next_term
        comparison_plot(f, u, Omega, 'tmp_sin%02dx' % i,
                        legend_loc='upper left', show=False,
                        plot_title='s=%g, i=%d' % (s, i))
```

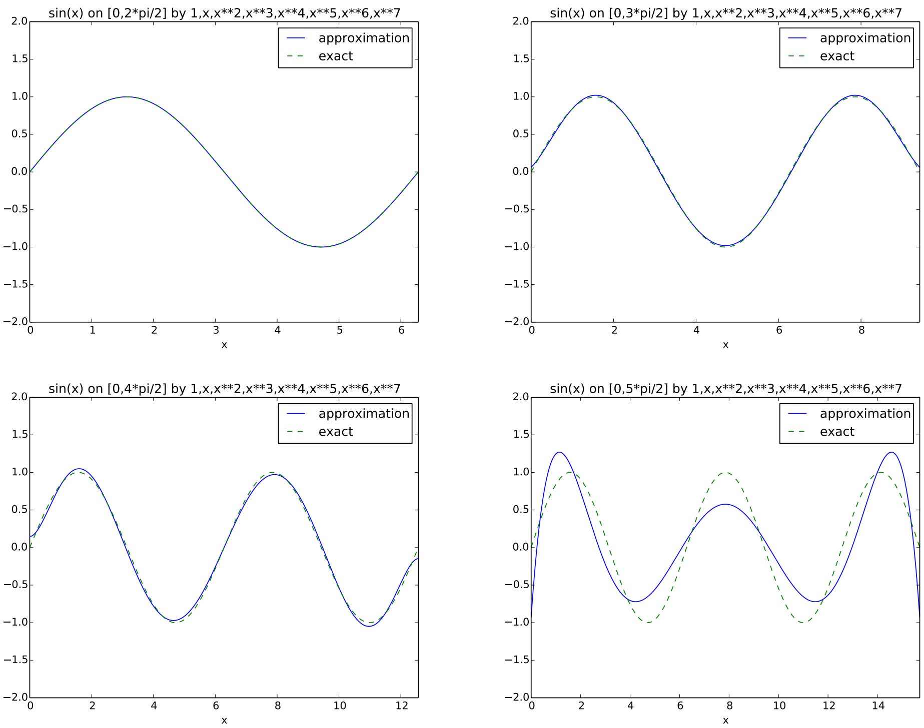


Figure 50: V_2 space, $\Omega_{1,k}$ domain.

```
if __name__ == '__main__':
    s = 20  # steepness
    f = sym.tanh(s*(x-sym.pi))
    from math import pi
    Omega = [0, 2*pi]  # sym.pi did not work here
    efficient(f, s, Omega, N=10)
    # Make movie
    # avconv/ffmpeg skips frames, use convert instead (few files)
    cmd = 'convert -delay 200 tmp_sin*.png tanh_sines_approx.gif'
    os.system(cmd)
    # Make static plots, 3 figures on 2 lines
    for ext in 'pdf', 'png':
        cmd = 'doconce combine_images %s -3 ' % ext
        cmd += 'tmp_sin00x tmp_sin01x tmp_sin02x tmp_sin04x '
        cmd += 'tmp_sin07x tmp_sin10x tanh_sines_approx'
        os.system(cmd)
    plt.show()
```

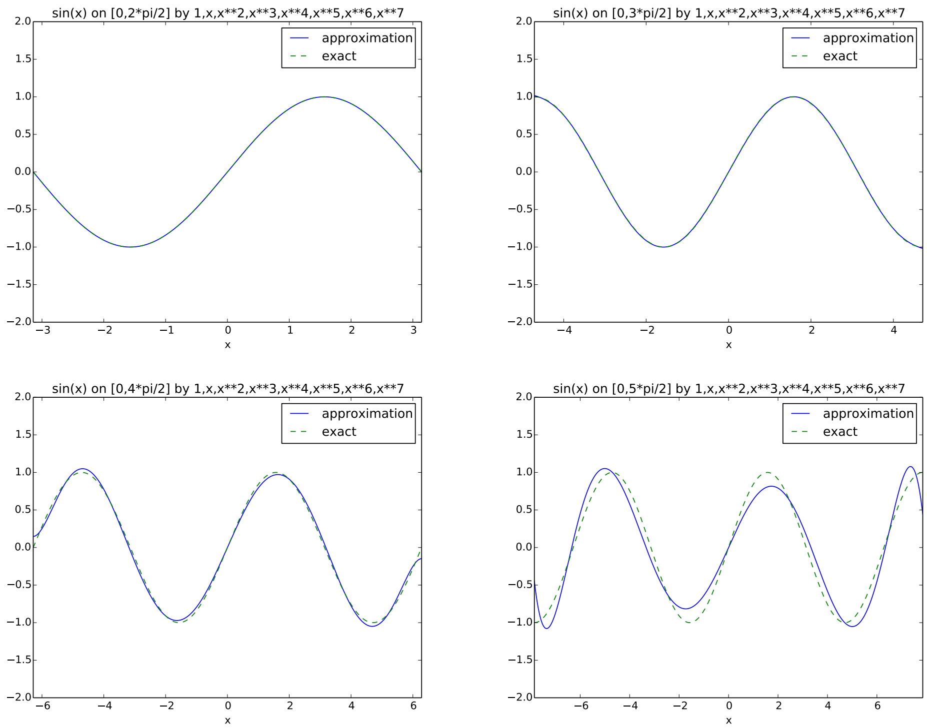
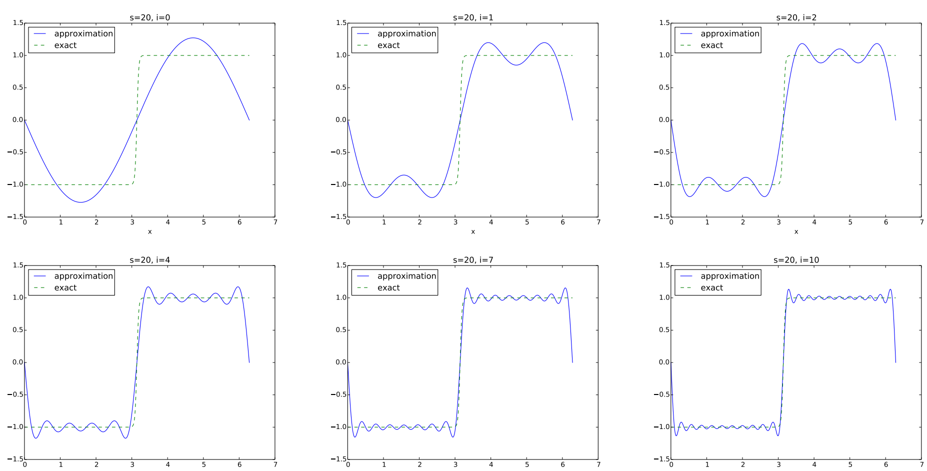


Figure 51: V_2 space, $\Omega_{2,k}$ domain.



Filename: `tanh_sines`.

Remarks. Approximation of a discontinuous (or steep) $f(x)$ by sines, results in slow convergence and oscillatory behavior of the approximation close to the abrupt changes in f. This is known as the Gibb's phenomenon.

Problem 7: Approximate a steep function by sines with boundary adjustment

We study the same approximation problem as in Problem 6. Since $\psi_i(0) = \psi_i(2\pi) = 0$ for all i, $u = 0$ at the boundary points $x = 0$ and $x = 2\pi$, while $f(0) = -1$ and $f(2\pi) = 1$. This discrepancy at the boundary can be removed by adding a boundary function $B(x)$:

$$u(x) = B(x) + \sum_{j\in\mathcal{I}_s} c_j\psi_j(x),$$

where $B(x)$ has the right boundary values: $B(x_L) = f(x_L)$ and $B(x_R) = f(x_R)$, with $x_L = 0$ and $x_R = 2\pi$ as the boundary points. A linear choice of $B(x)$ is

$$B(x) = \frac{(x_R - x)f(x_L) + (x - x_L)f(x_R)}{x_R - x_L}.$$

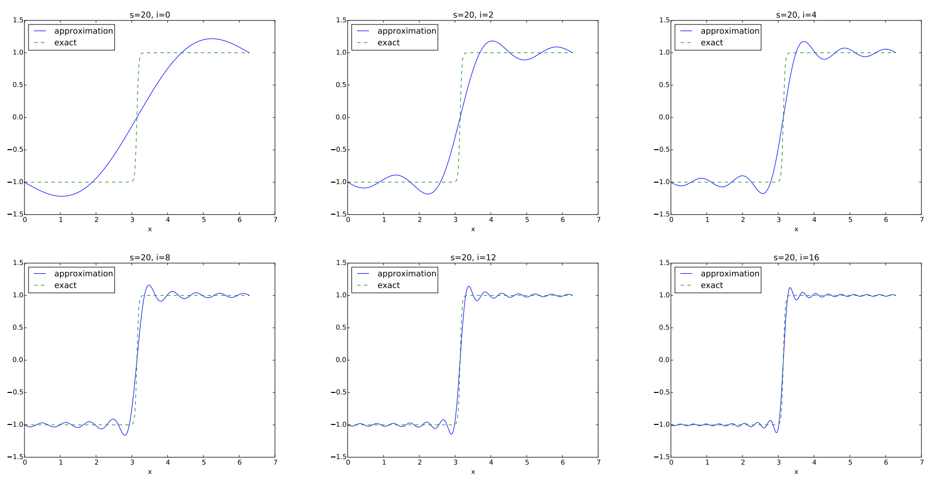
a) Use the basis $\psi_i(x) = \sin((i+1)x)$, $i \in \mathcal{I}_s = \{0,\ldots,N\}$ and plot u and f for $N = 16$. (It suffices to make plots for even i.)

Solution. With a boundary term $B(x)$ we call `least_squares_orth` with `f-B` as right-hand side function, and we must remember to add B to u.

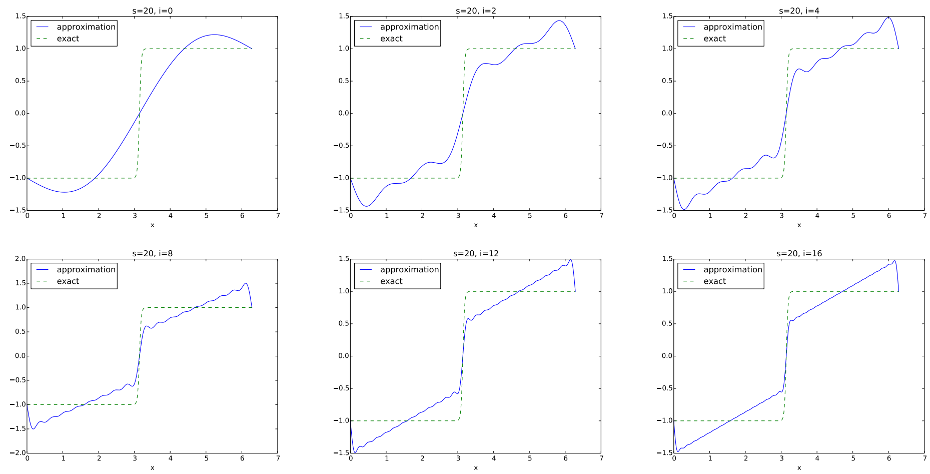
We can extend the code from Exercise 6 and let the function `efficient` handle different choices of basis. Appropriate code for all three subexercises is

```
import sympy as sym
from approx1D import least_squares_orth, comparison_plot
import matplotlib.pyplot as plt
import tanh_sines_approx
x = sym.Symbol('x')

def efficient(f, B, s, Omega, N=10, basis='a'):
    u = B
    for i in range(N+1):
        if basis == 'a':
            psi = [sym.sin((i+1)*x)]
        elif basis == 'b':
            psi = [sym.sin((2*i+1)*x)]
        elif basis == 'c':
            psi = [sym.sin(2*(i+1)*x)]
        next_term, c = least_squares_orth(f-B, psi, Omega, False)
        u = u + next_term
        # Make only plot for i even
        if i % 2 == 0:
            comparison_plot(f, u, Omega, 'tmp_sin%02dx' % i,
                            legend_loc='upper left', show=False,
                            plot_title='s=%g, i=%d' % (s, i))


if __name__ == '__main__':
```

```
    s = 20  # steepness
    f = sym.tanh(s*(x-sym.pi))
    from math import pi
    Omega = [0, 2*pi]  # sym.pi did not work here

    # sin((i+1)*x) basis
    xL = Omega[0]
    xR = Omega[1]
    B = ((xR-x)*f.subs(x, xL) + (x-xL)*f.subs(x, xR))/(xR-xL)
    for exercise in 'a', 'b', 'c':
        efficient(f, B, s, Omega, N=16, basis=exercise)
        # Make movie
        cmd = 'convert -delay 200 tmp_sin*.png '
        cmd += 'tanh_sines_boundary_term_%s.gif' % exercise
        os.system(cmd)
        # Make static plots, 3 figures on 2 lines
        for ext in 'pdf', 'png':
            cmd = 'doconce combine_images %s -3 ' % ext
            cmd += 'tmp_sin00x tmp_sin02x tmp_sin04x tmp_sin08x '
            cmd += 'tmp_sin12x tmp_sin16x '
            cmd += 'tanh_sines_boundary_term_%s' % exercise
            os.system(cmd)
```

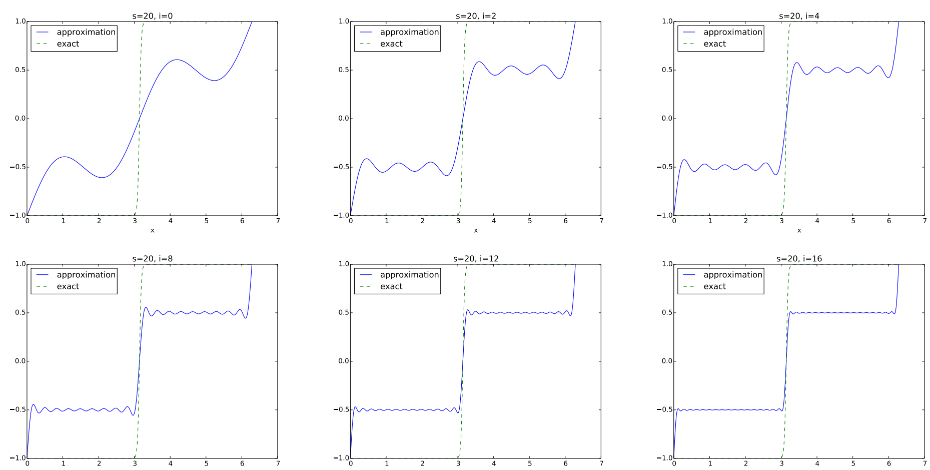


b) Use the basis from Exercise 6, $\psi_i(x) = \sin((2i+1)x)$, $i \in \mathcal{I}_s = \{0, \ldots, N\}$. (It suffices to make plots for even i.) Observe that the approximation converges to a piecewise linear function!



Solution.

c) Use the basis $\psi_i(x) = \sin(2(i+1)x)$, $i \in \mathcal{I}_s = \{0, \ldots, N\}$, and observe that the approximation converges to a piecewise constant function.



Solution. Filename: `tanh_sines_boundary_term`.

Remarks. The strange results in b) and c) are due to the choice of basis. In b), $\varphi_i(x)$ is an odd function around $x = \pi/2$ and $x = 3\pi/2$. No combination of basis functions is able to approximate the flat regions of f. All basis functions in c) are even around $x = \pi/2$ and $x = 3\pi/2$, but odd at $x = 0, \pi, 2\pi$. With all the sines represented, as in a), the approximation is not constrained with a particular symmetry behavior.

Exercise 8: Fourier series as a least squares approximation

a) Given a function $f(x)$ on an interval $[0, L]$, look up the formula for the coefficients a_j and b_j in the Fourier series of f:

$$f(x) = \frac{1}{2}a_0 + \sum_{j=1}^{\infty} a_j \cos\left(j\frac{2\pi x}{L}\right) + \sum_{j=1}^{\infty} b_j \sin\left(j\frac{2\pi x}{L}\right).$$

Solution. From Wikipedia we have

$$\begin{aligned}
a_j &= \frac{2}{L}\int_0^P f(x)\cos\left(j\frac{2\pi x}{L}\right)\,\mathrm{d}x,\\
b_j &= \frac{2}{L}\int_0^P f(x)\sin\left(j\frac{2\pi x}{L}\right)\,\mathrm{d}x\,.
\end{aligned}$$

b) Let an infinite-dimensional vector space V have the basis functions $\cos j\frac{2\pi x}{L}$ for $j = 0, 1, \ldots, \infty$ and $\sin j\frac{2\pi x}{L}$ for $j = 1, \ldots, \infty$. Show that the least squares approximation method from Section 2 leads to a linear system whose solution coincides with the standard formulas for the coefficients in a Fourier series of $f(x)$ (see also Section 2.7).

Hint. You may choose

$$\psi_{2i} = \cos\left(i\frac{2\pi}{L}x\right), \quad \psi_{2i+1} = \sin\left(i\frac{2\pi}{L}x\right), \tag{126}$$

for $i = 0, 1, \ldots, N \to \infty$.

Solution. The entries in the linear system arising from the least squares method are $A_{i,j} = \int_0^L \psi_i\psi_j\,\mathrm{d}x$ and $b_i = \int_0^L f(x)\psi_i\,\mathrm{d}x$. To avoid name clash between the right-hand side components of the linear system and the b_i coefficients in the Fourier series, we use the symbol q_i for the former. With the basis functions in (126) we get four different types of integrals:

$$
\begin{aligned}
A_{2i,2j} &= \int_0^L \cos\left(i\frac{2\pi}{L}x\right)\cos\left(j\frac{2\pi}{L}x\right)\,\mathrm{d}x = A_{2j,2i},\\
A_{2i,2j+1} &= \int_0^L \cos\left(i\frac{2\pi}{L}x\right)\sin\left(j\frac{2\pi}{L}x\right)\,\mathrm{d}x,\\
A_{2i+1,2j} &= \int_0^L \sin\left(i\frac{2\pi}{L}x\right)\cos\left(j\frac{2\pi}{L}x\right)\,\mathrm{d}x,\\
A_{2i+1,2j+1} &= \int_0^L \sin\left(i\frac{2\pi}{L}x\right)\sin\left(j\frac{2\pi}{L}x\right)\,dx,\\
q_{2i} &= \int_0^L f(x)\cos\left(i\frac{2\pi}{L}x\right)\,\mathrm{d}x,\\
q_{2i+1} &= \int_0^L f(x)\sin\left(i\frac{2\pi}{L}x\right)\,\mathrm{d}x\,.
\end{aligned}
$$

Now, the sine and cosine basis functions are orthogonal on $[0, L]$. We have in general

$$
\begin{aligned}
&\int_0^L \cos\left(i\frac{2\pi}{L}x\right)\cos\left(j\frac{2\pi}{L}x\right)\,\mathrm{d}x = 0, \quad i \neq j,\\
&\int_0^L \cos\left(i\frac{2\pi}{L}x\right)\cos\left(j\frac{2\pi}{L}x\right)\,\mathrm{d}x = \frac{L}{2}, \quad i = j \neq 0,\\
&\int_0^L \cos\left(i\frac{2\pi}{L}x\right)\cos\left(j\frac{2\pi}{L}x\right)\,\mathrm{d}x = L, \quad i = j = 0,\\
&\int_0^L \sin\left(i\frac{2\pi}{L}x\right)\sin\left(j\frac{2\pi}{L}x\right)\,\mathrm{d}x = 0, \quad i \neq j,\\
&\int_0^L \sin\left(i\frac{2\pi}{L}x\right)\sin\left(j\frac{2\pi}{L}x\right)\,\mathrm{d}x = \frac{L}{2}, \quad i = j,\\
&\int_0^L \cos\left(i\frac{2\pi}{L}x\right)\sin\left(j\frac{2\pi}{L}x\right)\,\mathrm{d}x = 0\,.
\end{aligned}
$$

These results imply that only diagonal terms in the coefficient matrix are different from zero. We have

$$
\begin{aligned}
A_{0,0} &= L,\\
A_{2i,2i} &= \frac{L}{2}, \quad i > 0,\\
A_{2i+1,2i+1} &= \frac{L}{2}\,.
\end{aligned}
$$

The unknown vector with components c_i must be arranged as

$$(a_0, b_1, a_1, b_2, a_2, b_3, \ldots)\,.$$

We then get

$$A_{0,0}a_0 = q_0, \quad A_{1,1}b_1 = q_1, \quad A_{2,2}a_1 = q_2, \quad A_{3,3}b_2 = q_3, \ldots$$

These equations lead to the formulas

$$\begin{aligned}
a_0 &= \frac{1}{L}\int_0^P f(x)\,\mathrm{d}x,\\
b_1 &= \frac{2}{L}\int_0^P f(x)\sin\left(\frac{2\pi}{L}x\right)\,\mathrm{d}x,\\
a_1 &= \frac{2}{L}\int_0^P f(x)\cos\left(\frac{2\pi}{L}x\right)\,\mathrm{d}x,\\
b_2 &= \frac{2}{L}\int_0^P f(x)\sin\left(2\frac{2\pi}{L}x\right)\,\mathrm{d}x,\\
a_2 &= \frac{2}{L}\int_0^P f(x)\cos\left(2\frac{2\pi}{L}x\right)\,\mathrm{d}x\,.
\end{aligned}$$

which can be generalized to

$$\begin{aligned}
a_0 &= \frac{1}{L}\int_0^P f(x)\,\mathrm{d}x,\\
a_j &= \frac{2}{L}\int_0^P f(x)\cos\left(j\frac{2\pi}{L}x\right)\,\mathrm{d}x,\ j > 0,\\
b_j &= \frac{2}{L}\int_0^P f(x)\sin\left(j\frac{2\pi}{L}x\right)\,\mathrm{d}x,\ j > 0,
\end{aligned}$$

and these are the standard formulas for the Fourier coefficients in a) if we recognize that the a_0 above is twice the a_0 in the expressions in a).

c) Choose $f(x) = H(x - \frac{1}{2})$ on $\Omega = [0, 1]$, where H is the Heaviside function: $H(x) = 0$ for $x < 0$, $H(x) = 1$ for $x > 0$ and $H(0) = \frac{1}{2}$. Find the coefficients a_j and b_j in the Fourier series for $f(x)$. Plot the sum for $j = 2N + 1$, where $N = 5$ and $N = 100$.

Solution. The formulas give

$$
\begin{aligned}
a_0 &= 2\int_0^1 f(x)\,\mathrm{d}x = 2\int_{\frac{1}{2}}^1 \mathrm{d}x,\\
a_j &= 2\int_0^1 f(x)\cos\left(2j\pi x\right)\,\mathrm{d}x = 2\int_{\frac{1}{2}}^1 \cos\left(2j\pi x\right)\,\mathrm{d}x,\\
b_j &= 2\int_{\frac{1}{2}}^1 \sin\left(2j\pi x\right)\,\mathrm{d}x\,.
\end{aligned}
$$

The integrals are readily computed by `sympy`:

```
>>> import sympy as sym
>>> j = sym.symbols('k', integer=True)
>>> x = sym.symbols('x', real=True)
>>> I = integrate(cos(2*j*pi*x), (x,Rational(1,2),1))
>>> I
0
>>> I = integrate(cos(2*0*pi*x), (x,Rational(1,2),1))
>>> I
1/2
>>> I = integrate(sin(2*j*pi*x), (x,Rational(1,2),1))
>>> I
(-1)**j/(2*pi*j) - 1/(2*pi*j)
```

This means that we have the series

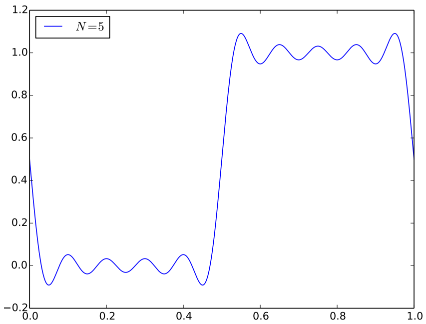
$$
u(x) = \frac{1}{2} + 2\sum_{j=1}^{\infty}\frac{(-1)^j - 1}{2\pi j}\sin\left(2j\pi x\right)\,.
$$

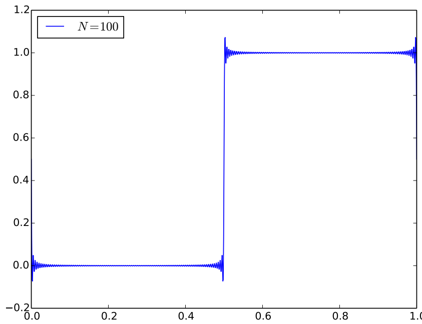
We only get a nonzero coefficient for j odd:

$$
u(x) = \frac{1}{2} - 2\sum_{k=1}^{\infty}\frac{1}{(2k+1)\pi}\sin\left(2(2k+1)\pi x\right)\,.
$$

Appropriate computer code for visualizing the series goes like

```
import numpy as np
import matplotlib.pyplot as plt
from math import pi
from numpy import sin

def Heaviside_series(x, N):
    s = 0.5
    for k in range(N):
        s += -2.0/((2*k+1)*pi)*sin(2*(2*k+1)*pi*x)
    return s

x = np.linspace(0, 1, 1001)
for N in 5, 100:
    H = Heaviside_series(x, N)
    plt.figure()
    plt.plot(x, H)
    plt.legend(['$N=%d$' % N], loc='upper left')
    plt.savefig('tmp_%d.png' % N)
    plt.savefig('tmp_%d.pdf' % N)
plt.show()
```





We clearly see the Gibbs' phenomenon: oscillations and overshoot around the point of discontinuity in the function we try to approximate.
Filename: `Fourier_ls`.

Problem 9: Approximate a steep function by Lagrange polynomials

Use interpolation with uniformly distributed points and Chebychev nodes to approximate

$$f(x) = -\tanh(s(x - \frac{1}{2})), \quad x \in [0, 1],$$

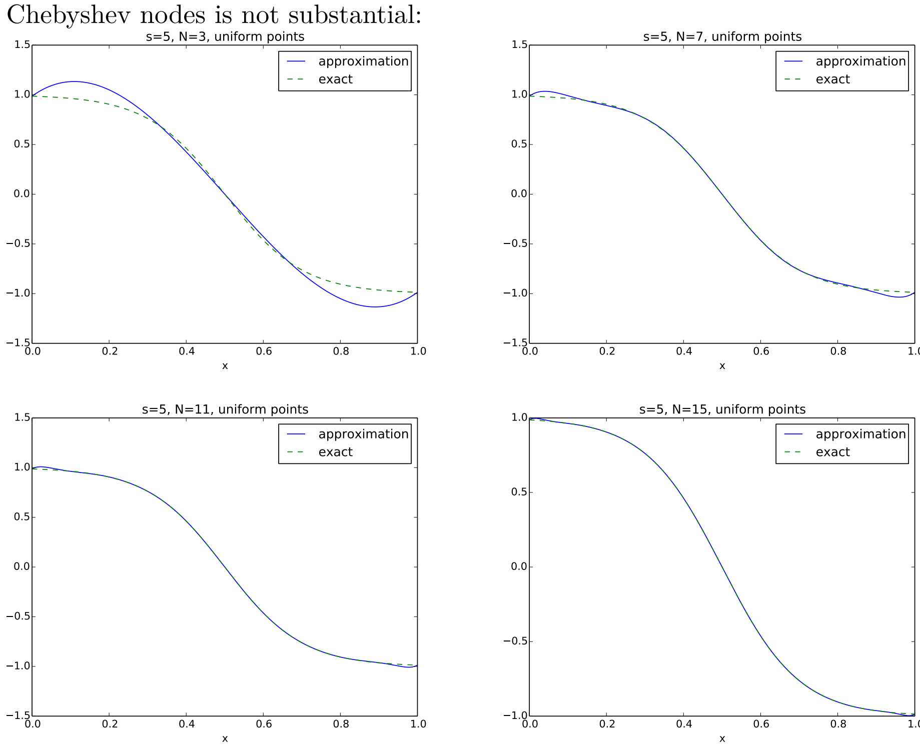
by Lagrange polynomials for $s = 5$ and $s = 20$, and $N = 3, 7, 11, 15$. Combine 2×2 plots of the approximation for the four N values, and create such figures for the four combinations of s values and point types.

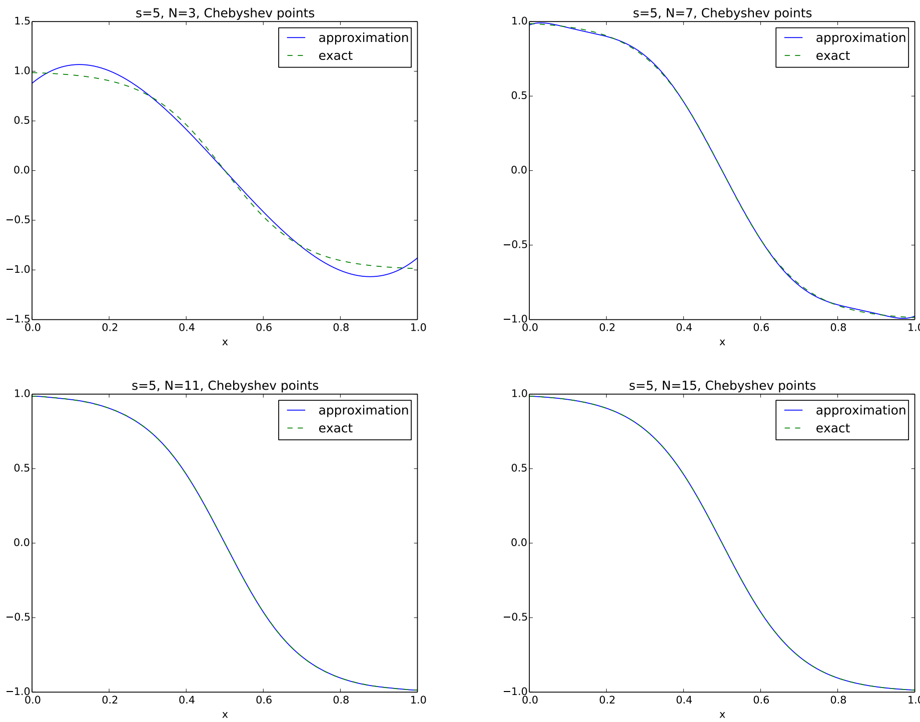
Solution. The following code does the work (symbolically):

```
import sys, os
sys.path.insert(0, os.path.join(os.pardir, 'src-approx'))
from approx1D import interpolation, comparison_plot
from Lagrange import Lagrange_polynomials
import sympy as sym

x = sym.Symbol('x')
Omega = [0,1]
N_values = 3, 7, 11, 15

for s in 5, 20:
    f = -sym.tanh(s*(x-0.5))  # sympy expression
    for distribution in 'uniform', 'Chebyshev':
        for N in N_values:
            phi, points = Lagrange_polynomials(
                x, N, Omega,
                point_distribution=distribution)

            u, c = interpolation(f, phi, points)
            filename = 'tmp_tanh_%d_%d_%s' % (N, s, distribution)
            comparison_plot(f, u, Omega, filename,
                            plot_title='s=%g, N=%d, %s points' %
                            (s, N, distribution))
        # Combine plot files (2x2)
        for ext in 'png', 'pdf':
```

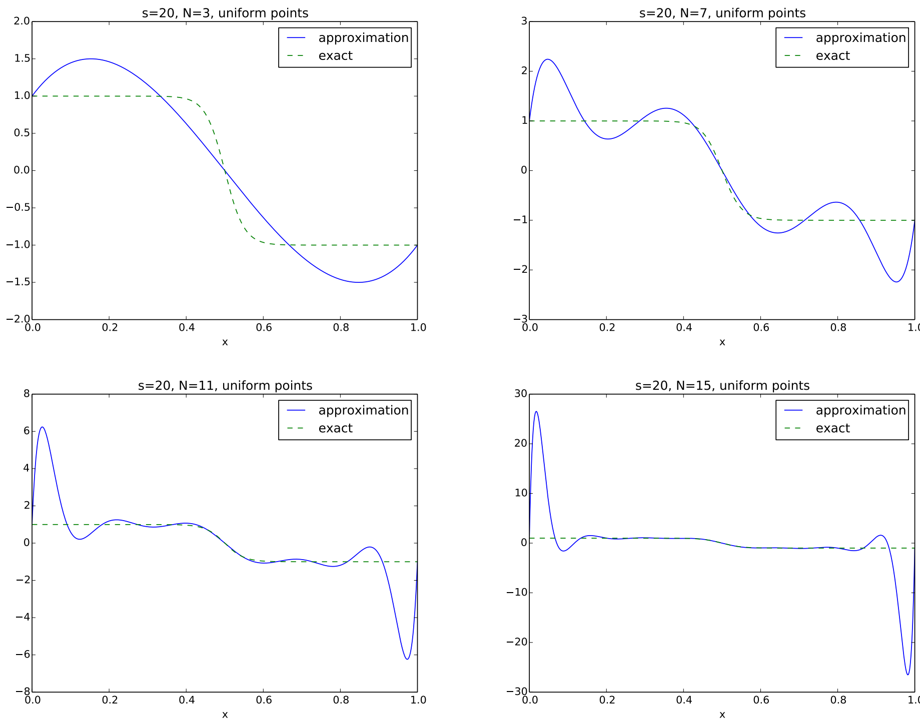
```
            cmd = 'doconce combine_images ' + ext + ' '
            cmd += ' '.join([
                'tmp_tanh_%d_%d_%s' % (N, s, distribution)
                for N in N_values])
            cmd += ' tanh_Lagrange_%s_s%s' % (distribution, s)
            os.system(cmd)
```

For a smooth function ($s = 5$), the difference between uniform points and Chebyshev nodes is not substantial:

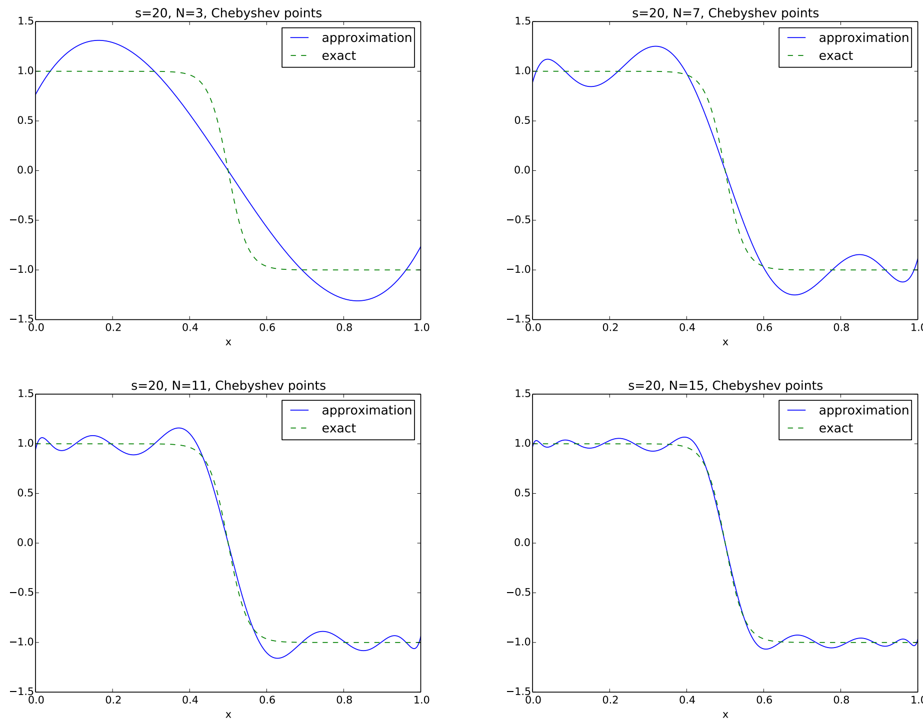




However, for a steep function ($s = 20$) the overshoot and oscillations associated with uniform points must be considered unacceptable for larger N values:



Switching to Chebyshev points does give a great improvement, but we still have oscillatory approximations:



Filename: `tanh_Lagrange`.

Problem 10: Approximate a steep function by Lagrange polynomials and regression

Redo Problem 9, but apply a regression method with N-degree Lagrange polynomials and $2N+1$ data points. Recall that Problem 9 applies $N+1$ points and the resulting approximation interpolates f at these points, while a regression method with more points does not interpolate f at the data points. Do more points and a regression method help reduce the oscillatory behavior of Lagrange polynomial approximations?

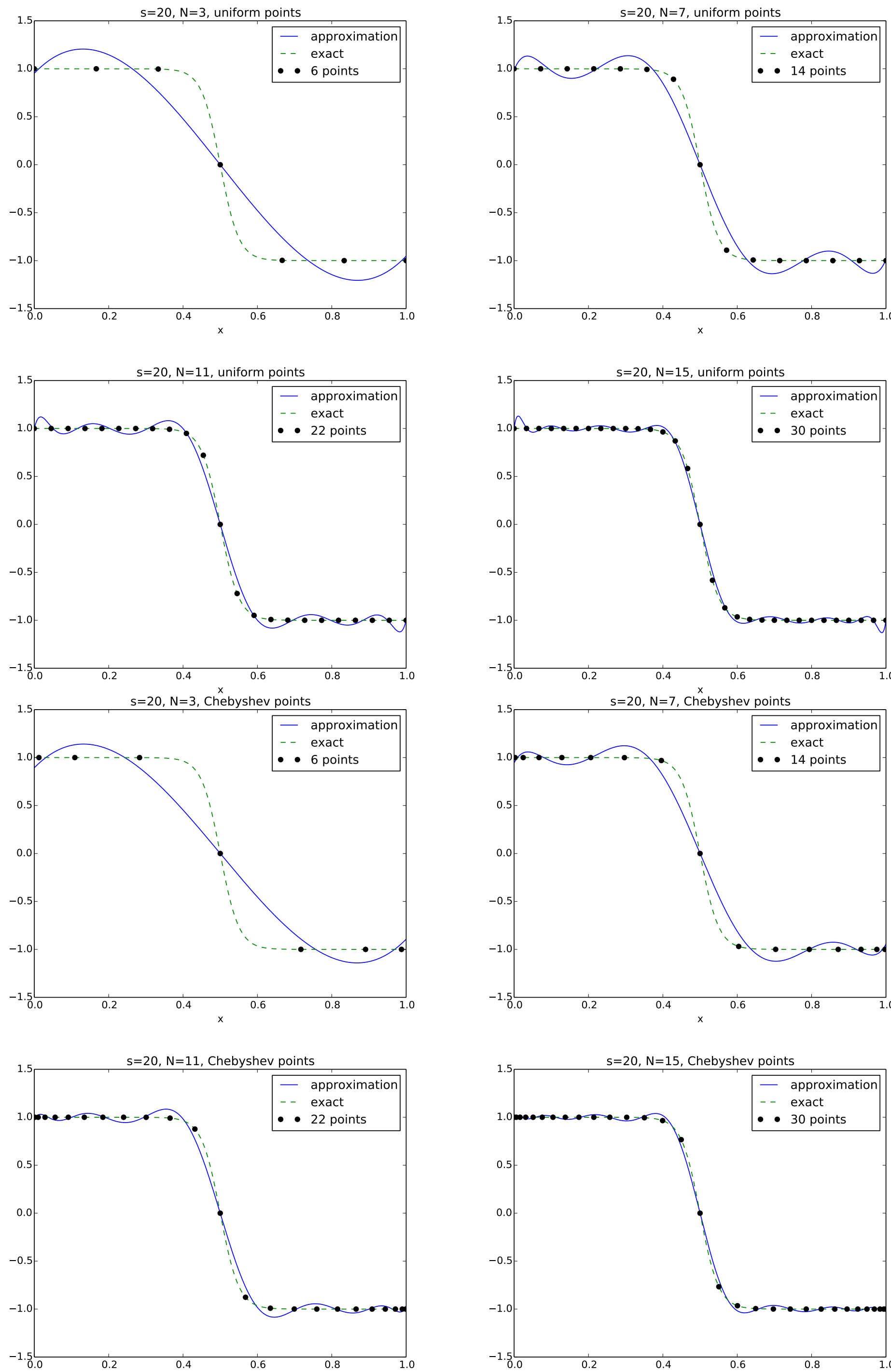
Solution. We start out with the program from Problem 9. This time we need to call `Lagrange_polynomails` twice: first to compute the $\psi(x)$ functions (of degree N) and then to compute the data points corresponding to a uniform or Chebyshev distribution of $2N+1$ nodes.

```
import sys, os
sys.path.insert(0, os.path.join(os.pardir, 'src-approx'))
from approx1D import regression, comparison_plot
from Lagrange import Lagrange_polynomials
import sympy as sym
import numpy as np

x = sym.Symbol('x')
```

```
Omega = [0,1]
N_values = 3, 7, 11, 15

for s in 5, 20:
    f = -sym.tanh(s*(x-0.5))  # sympy expression
    for distribution in 'uniform', 'Chebyshev':
        for N in N_values:
            # Compute the points from a 2*N Lagrange polynomial
            dummy, points = Lagrange_polynomials(
                x, 2*N, Omega,
                point_distribution=distribution)
            # Compute phi from N points Lagrange polynomial
            phi, dummy = Lagrange_polynomials(
                x, N, Omega,
                point_distribution=distribution)
            points = np.array(points, dtype=float)
            point_values = -np.tanh(s*(points-0.5))

            u, c = regression(f, phi, points)
            filename = 'tmp_tanh_%d_%d_%s' % (N, s, distribution)
            comparison_plot(f, u, Omega, filename,
                            plot_title='s=%g, N=%d, %s points' %
                            (s, N, distribution),
                            points=points, point_values=point_values,
                            points_legend='%s points' % (2*N))
        # Combine plot files (2x2)
        for ext in 'png', 'pdf':
            cmd = 'doconce combine_images ' + ext + ' '
            cmd += ' '.join([
                'tmp_tanh_%d_%d_%s' % (N, s, distribution)
                for N in N_values])
            cmd += ' tanh_Lagrange_regr_%s_s%s' % (distribution, s)
            os.system(cmd)
```

An important point is to convert `points` to a `numpy` array using `dtype=float`. Leaving out this second argument makes an array of objects of symbolic expressions, and we cannot apply `tanh` to it.

The oscillatory behavior is much reduced using more points and a regression method, and the difference between uniform and Chebyshev points is minor, even in the steep case $s = 20$:



Filename: `tanh_Lagrange_regression`.

Problem 11: Define nodes and elements

Consider a domain $\Omega = [0, 2]$ divided into the three elements $[0, 1]$, $[1, 1.2]$, and $[1.2, 2]$.

For P1 and P2 elements, set up the list of coordinates and nodes (`nodes`) and the numbers of the nodes that belong to each element (`elements`) in two cases: 1) nodes and elements numbered from left to right, and 2) nodes and elements numbered from right to left.

Solution. We can write up figure sketches and the data structure in code:

```
# P1 elements
# Left to right numbering
"""
elements: |--0--|--1--|--2--|
nodes:    0     1     2     3
"""

nodes    = [0, 1, 1.2, 2]
elements = [[0,1], [1,2], [2,3]]

# Right to left numbering
"""
elements: |--2--|--1--|--0--|
nodes:    3     2     1     0
"""

nodes    = [2, 1.2, 1, 0]
elements = [[1,0], [2,1], [3,2]]


# P2 elements

# Left to right numbering
"""
elements: |--0--|--1--|--2--|
nodes:    0  1  2  3  4  5  6
"""

nodes = [0, 0.5, 1, 1.1, 1.6, 2]
elements = [[0,1,2], [2,3,4], [4,5,6]]

# Right to left numbering
"""
elements: |--2--|--1--|--0--|
nodes:    6  5  4  3  2  1  0
"""

nodes = [2, 1.6, 1.2, 1.1, 1, 0.5, 0]
elements = [[2,1,0], [4,3,2], [6,5,4]]
```

Filename: `fe_numberings1`.

Problem 12: Define vertices, cells, and dof maps

Repeat Problem 11, but define the data structures `vertices`, `cells`, and `dof_map` instead of `nodes` and `elements`.

Solution. Written in Python, the solution becomes

```
# P1 elements
# Left to right numbering
"""
elements: |--0--|--1--|--2--|
vertices: 0     1     2     3
dofs:     0     1     2     3
"""
# elements:   0   1   2
# vertices: 0   1   2   3

vertices = [0, 1, 1.2, 2]
cells    = [[0,1], [1,2], [2,3]]
dof_map  = [[0,1], [1,2], [2,3]]

# Right to left numbering
"""
elements: |--2--|--1--|--0--|
vertices: 3     2     1     0
dofs:     3     2     1     0
"""

vertices = [2, 1.2, 1, 0]
cells    = [[1,0], [2,1], [3,2]]
dof_map  = [[1,0], [2,1], [3,2]]


# P2 elements

# Left to right numbering
# elements:   0   1   2
"""
elements: |--0--|--1--|--2--|
vertices: 0     1     2     3
dofs:     0  1  2  3  4  5  6
"""

vertices = [0, 1, 1.2, 2]
cells    = [[0,1], [1,2], [2,3]]
dof_map  = [[0,1,2], [2,3,4], [4,5,6]]

# Right to left numbering
# elements:   2   1   0
"""
elements: |--2--|--1--|--0--|
vertices: 3     2     1     0
dofs:     6  5  4  3  2  1  0
"""

vertices = [2, 1.2, 1, 0]
cells    = [[1,0], [2,1], [3,2]]
dof_map  = [[2,1,0], [4,3,2], [6,5,4]]
```

Filename: `fe_numberings2`.

Problem 13: Construct matrix sparsity patterns

Problem 11 describes a element mesh with a total of five elements, but with two different element and node orderings. For each of the two orderings, make a 5×5 matrix and fill in the entries that will be nonzero.

Hint. A matrix entry (i, j) is nonzero if i and j are nodes in the same element.

Solution. If we create an empty matrix, we can run through all elements and then over all local node pairs and mark that the corresponding entry (i, j) in the global matrix is a nonzero entry. The `elements` data structure is sufficient. Below is a program that fills matrix entries with an `X` and prints the matrix sparsity pattern.

```
def sparsity_pattern(elements, N_n):
    import numpy as np
    matrix = np.zeros((N_n, N_n), dtype=str)
    matrix[:,:] = '0'
    for e in elements:
        for i in e:
            for j in e:
                matrix[i,j] = 'X'
    matrix = matrix.tolist()
    matrix = '\n'.join([' '.join([matrix[i][j]
                                  for j in range(len(matrix[i]))])
                        for i in range(len(matrix))])
    return matrix


print '\nP1 elements, left-to-right numbering'
N_n = 4
elements = [[0,1], [1,2], [2,3]]
print sparsity_pattern(elements, N_n)

print '\nP1 elements, right-to-left numbering'
elements = [[1,0], [2,1], [3,2]]
print sparsity_pattern(elements, N_n)

print '\nP2 elements, left-to-right numbering'
N_n = 7
elements = [[0,1,2], [2,3,4], [4,5,6]]
print sparsity_pattern(elements, N_n)

print '\nP1 elements, right-to-left numbering'
elements = [[2,1,0], [4,3,2], [6,5,4]]
print sparsity_pattern(elements, N_n)
```

The output becomes

```
P1 elements, left-to-right numbering
X X 0 0
X X X 0
0 X X X
0 0 X X

P1 elements, right-to-left numbering
X X 0 0
X X X 0
0 X X X
0 0 X X

P2 elements, left-to-right numbering
X X X 0 0 0 0
X X X 0 0 0 0
X X X X X 0 0
```

```
0 0 X X X 0 0
0 0 X X X X X
0 0 0 0 X X X
0 0 0 0 X X X

P1 elements, right-to-left numbering
X X X 0 0 0 0
X X X 0 0 0 0
X X X X X 0 0
0 0 X X X 0 0
0 0 X X X X X
0 0 0 0 X X X
0 0 0 0 X X X
```

Filename: `fe_sparsity_pattern`.

Problem 14: Perform symbolic finite element computations

Perform symbolic calculations to find formulas for the coefficient matrix and right-hand side when approximating $f(x) = \sin(x)$ on $\Omega = [0, \pi]$ by two P1 elements of size $\pi/2$. Solve the system and compare $u(\pi/2)$ with the exact value 1.

Solution. Here are suitable `sympy` commands:

```
import sympy as sym
# Mesh: |--------|-------|
#       0      pi/2      pi
#
# Basis functions:
#
#   phi_0   phi_1   phi_2
#     \      /\      /
#      \    /  \    /
#       \  /    \  /
#        \/      \/
#     |-------|-------|
#     0      pi/2     pi

x = sym.Symbol('x')
A = sym.zeros((3,3))
f = sym.sin

phi_0 = 1 - (2*x)/sym.pi
phi_1l = 2*x/sym.pi          # left part of phi_1
phi_1r = 2 - (2*x)/sym.pi    # right part of phi_1
phi_2 = x/(sym.pi/2) - 1
node_0 = 0
node_1 = sym.pi/2
node_2 = sym.pi

# Diagonal terms
A[0,0] = sym.integrate(phi_0**2,  (x, node_0, node_1))
A[1,1] = sym.integrate(phi_1l**2, (x, node_0, node_1)) + \
         sym.integrate(phi_1r**2, (x, node_1, node_2))
A[2,2] = sym.integrate(phi_2**2,  (x, node_1, node_2))

# Off-diagonal terms
A[0,1] = sym.integrate(phi_0*phi_1l, (x, node_0, node_1))
```

```
A[1,0] = A[0,1]

A[1,2] = sym.integrate(phi_1r*phi_2, (x, node_1, node_2))
A[2,1] = A[1,2]

print 'A:\n', A  # Can compare with general matrix, h=pi/2

b = sym.zeros((3,1))

b[0] = sym.integrate(phi_0*f(x),  (x, node_0, node_1))
b[1] = sym.integrate(phi_1l*f(x), (x, node_0, node_1)) + \
       sym.integrate(phi_1r*f(x), (x, node_1, node_2))
b[2] = sym.integrate(phi_2*f(x),  (x, node_1, node_2))

print 'b:\n', b

c = A.LUsolve(b)
print 'c:\n', c

for i in range(len(c)):
    print 'c[%d]=%g' % (i, c[i].evalf())
print 'u(pi/2)=%g' % c[1]

# For reports
print sym.latex(A)
print sym.latex(b)
print sym.latex(c)
```

Running the program, we get the matrix system

$$\left[\begin{matrix}\frac{\pi}{6} & \frac{\pi}{12} & 0\\\frac{\pi}{12} & \frac{\pi}{3} & \frac{\pi}{12}\\0 & \frac{\pi}{12} & \frac{\pi}{6}\end{matrix}\right]\left[\begin{matrix}\frac{1}{\pi} \left(- \frac{24}{\pi} + 8\right)\\\frac{-28 + \frac{168}{\pi}}{7 \pi}\\\frac{1}{\pi} \left(- \frac{24}{\pi} + 8\right)\end{matrix}\right] = \left[\begin{matrix}- \frac{2}{\pi} + 1\\\frac{4}{\pi}\\- \frac{2}{\pi} + 1\end{matrix}\right]$$

The solution at the midpoint is 1.15847, i.e., 16% error.
Filename: `fe_sin_P1`.

Problem 15: Approximate a steep function by P1 and P2 elements

Given

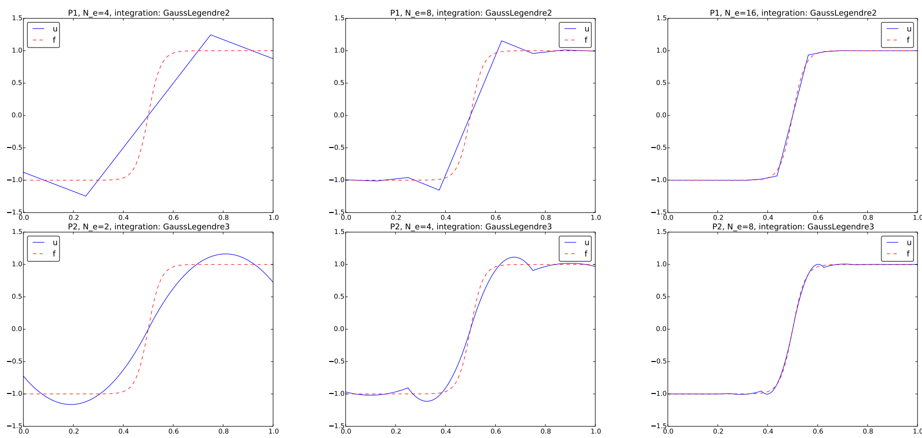
$$f(x) = \tanh(s(x - \frac{1}{2}))$$

use the Galerkin or least squares method with finite elements to find an approximate function $u(x)$. Choose $s = 20$ and try $N_e = 4, 8, 16$ P1 elements and $N_e = 2, 4, 8$ P2 elements. Integrate $f\varphi_i$ numerically.

Hint. You can automate the computations by calling the `approximate` method in the `fe_approx1D_numint` module.

Solution. The set of calls to `approximate` becomes

```
from fe_approx1D_numint import approximate
from sympy import tanh, Symbol
x = Symbol('x')

steepness = 20
arg = steepness*(x-0.5)
approximate(tanh(arg), symbolic=False, numint='GaussLegendre2',
            d=1, N_e=4, filename='fe_p1_tanh_4e')
approximate(tanh(arg), symbolic=False, numint='GaussLegendre2',
            d=1, N_e=8, filename='fe_p1_tanh_8e')
approximate(tanh(arg), symbolic=False, numint='GaussLegendre2',
            d=1, N_e=16, filename='fe_p1_tanh_16e')
approximate(tanh(arg), symbolic=False, numint='GaussLegendre3',
            d=2, N_e=2, filename='fe_p2_tanh_2e')
approximate(tanh(arg), symbolic=False, numint='GaussLegendre3',
            d=2, N_e=4, filename='fe_p2_tanh_4e')
approximate(tanh(arg), symbolic=False, numint='GaussLegendre3',
            d=2, N_e=8, filename='fe_p2_tanh_8e')
```



Filename: `fe_tanh_P1P2`.

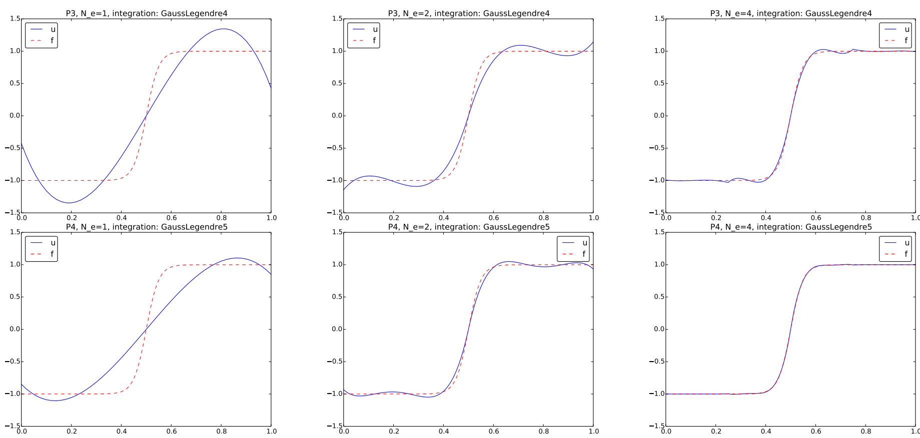
Problem 16: Approximate a steep function by P3 and P4 elements

a) Solve Problem 15 using $N_e = 1, 2, 4$ P3 and P4 elements.

Solution. We can easily adopt the code from Exercise 15:

```
from fe_approx1D_numint import approximate, u_glob
from sympy import tanh, Symbol, lambdify
x = Symbol('x')

steepness = 20
arg = steepness*(x-0.5)

approximate(tanh(arg), symbolic=False, numint='GaussLegendre4',
            d=3, N_e=1, filename='fe_p3_tanh_1e')
approximate(tanh(arg), symbolic=False, numint='GaussLegendre4',
            d=3, N_e=2, filename='fe_p3_tanh_2e')
approximate(tanh(arg), symbolic=False, numint='GaussLegendre4',
```

```
              d=3, N_e=4, filename='fe_p3_tanh_4e')
approximate(tanh(arg), symbolic=False, numint='GaussLegendre5',
              d=4, N_e=1, filename='fe_p4_tanh_1e')
approximate(tanh(arg), symbolic=False, numint='GaussLegendre5',
              d=4, N_e=2, filename='fe_p4_tanh_2e')
approximate(tanh(arg), symbolic=False, numint='GaussLegendre5',
              d=4, N_e=4, filename='fe_p4_tanh_4e')
```

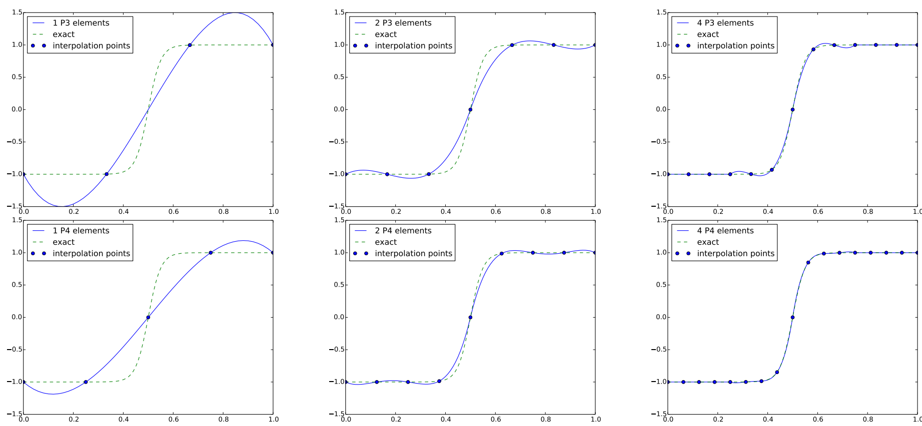


b) How will an interpolation method work in this case with the same number of nodes?

Solution. The coefficients arising from the interpolation method are trivial to compute since $c_i = f(x_i)$, where x_i are the global nodes. The function `u_glob` in the `fe_approx1D_numint` module can be used to compute appropriate arrays for plotting the resulting finite element function. We create plots where the finite element approximation is shown along with $f(x)$ and the interpolation points. Since `u_glob` requires the `vertices`, `cells`, and `dof_map` data structures, we must compute these for the values of number of elements (N_e) and the polynomial degree (d).

```
# Interpolation method
import numpy as np
import matplotlib.pyplot as plt
f = lambdify([x], tanh(arg), modules='numpy')

# Compute exact f on a fine mesh
x_fine = np.linspace(0, 1, 101)
f_fine = f(x_fine)

for d in 3, 4:
    for N_e in 1, 2, 4:
        h = 1.0/N_e  # element length
        vertices = [i*h for i in range(N_e+1)]
        cells = [[e, e+1] for e in range(N_e)]
        dof_map = [[d*e + i for i in range(d+1)] for e in range(N_e)]
        N_n = d*N_e + 1  # Number of nodes
        x_nodes = np.linspace(0, 1, N_n)  # Node coordinates
        U = f(x_nodes)  # Interpolation method samples node values
        x, u = u_glob(U, vertices, cells, dof_map,
```

```
                        resolution_per_element=51)
          plt.figure()
          plt.plot(x, u, '-', x_fine, f_fine, '--',
                   x_nodes, U, 'bo')
          plt.legend(['%d P%d elements' % (N_e, d),
                      'exact', 'interpolation points'],
                     loc='upper left')
          plt.savefig('tmp_%d_P%d.pdf' % (N_e, d))
          plt.savefig('tmp_%d_P%d.png' % (N_e, d))
  plt.show()
```



Filename: `fe_tanh_P3P4`.

Exercise 17: Investigate the approximation error in finite elements

The theory (102) from Section 6.4 predicts that the error in the Pd approximation of a function should behave as h^{d+1}, where h is the length of the element. Use experiments to verify this asymptotic behavior (i.e., for small enough h). Choose three examples: $f(x) = Ae^{-\omega x}$ on $[0, 3/\omega]$, $f(x) = A\sin(\omega x)$ on $\Omega = [0, 2\pi/\omega]$ for constant A and ω, and $f(x) = \sqrt{x}$ on $[0, 1]$.

Hint. Run a series of experiments: (h_i, E_i), $i = 0, \ldots, m$, where E_i is the L^2 norm of the error corresponding to element length h_i. Assume an error model $E = Ch^r$ and compute r from two successive experiments:

$$r_i = \ln(E_{i+1}/E_i)/\ln(h_{i+1}/h_i), \quad i = 0, \ldots, m-1\,.$$

Hopefully, the sequence $r_0, \ldots, r_{m-1}$ converges to the true r, and r_{m-1} can be taken as an approximation to r. Run such experiments for different d for the different $f(x)$ functions.
Filename: `Pd_approx_error`.

Problem 18: Approximate a step function by finite elements

Approximate the step function

$$f(x) = \begin{cases} 1 & 0 \leq x < 1/2, \\ 2 & 1/2 \leq x \geq 1/2 \end{cases}$$

by 2, 4, and 8 P1 and P2 elements. Compare approximations visually.

Hint. This f can also be expressed in terms of the Heaviside function $H(x)$: $f(x) = H(x - 1/2)$. Therefore, f can be defined by

```
f = sym.Heaviside(x - sym.Rational(1,2))
```

making the `approximate` function in the `fe_approx1D.py` module an obvious candidate to solve the problem. However, `sympy` does not handle symbolic integration with this particular integrand, and the `approximate` function faces a problem when converting `f` to a Python function (for plotting) since `Heaviside` is not an available function in `numpy`. It is better to make special-purpose code for this case or perform all calculations by hand.
Filename: `fe_Heaviside_P1P2`.

Exercise 19: 2D approximation with orthogonal functions

Assume we have basis functions $\varphi_i(x, y)$ in 2D that are orthogonal such that $(\varphi_i, \varphi_j) = 0$ when $i \neq j$. The function `least_squares` in the file `approx2D.py` will then spend much time on computing off-diagonal terms in the coefficient matrix that we know are zero. To speed up the computations, make a version `least_squares_orth` that utilizes the orthogonality among the basis functions. Apply the function to approximate

$$f(x, y) = x(1 - x)y(1 - y)e^{-x-y}$$

on $\Omega = [0, 1] \times [0, 1]$ via basis functions

$$\varphi_i(x, y) = \sin((p + 1)\pi x) \sin((q + 1)\pi y), \quad i = q(N_x + 1) + p,$$

where $p = 0, \ldots, N_x$ and $q = 0, \ldots, N_y$.

Hint. Get ideas from the function `least_squares_orth` in Section 2.8 and file `approx1D.py`.
Filename: `approx2D_ls_orth`.

Exercise 20: Use the Trapezoidal rule and P1 elements

Consider approximation of some $f(x)$ on an interval Ω using the least squares or Galerkin methods with P1 elements. Derive the element matrix and vector using the Trapezoidal rule (110) for calculating integrals on the reference element. Assemble the contributions, assuming a uniform cell partitioning, and show that the resulting linear system has the form $c_i = f(x_i)$ for $i \in \mathcal{I}_s$. Filename: `fe_P1_trapez`.

Exercise 21: Compare P1 elements and interpolation

We shall approximate the function

$$f(x) = 1 + \epsilon \sin(2\pi n x), \quad x \in \Omega = [0, 1],$$

where $n \in \mathbb{Z}$ and $\epsilon \geq 0$.

a) Plot $f(x)$ for $n = 1, 2, 3$ and find the wave length of the function.

b) We want to use N_P elements per wave length. Show that the number of elements is then nN_P.

c) The critical quantity for accuracy is the number of elements per wave length, not the element size in itself. It therefore suffices to study an f with just one wave length in $\Omega = [0, 1]$. Set $\epsilon = 0.5$.

Run the least squares or projection/Galerkin method for $N_P = 2, 4, 8, 16, 32$. Compute the error $E = ||u - f||_{L^2}$.

Hint. Use the `fe_approx1D_numint` module to compute u and use the technique from Section 6.4 to compute the norm of the error.

d) Repeat the set of experiments in the above point, but use interpolation/collocation based on the node points to compute $u(x)$ (recall that c_i is now simply $f(x_i)$). Compute the error $E = ||u - f||_{L^2}$. Which method seems to be most accurate? Filename: `fe_P1_vs_interp`.

Exercise 22: Implement 3D computations with global basis functions

Extend the `approx2D.py` code to 3D applying ideas from Section 8.4. Use a 3D generalization of the test problem in Section 8.3 to test the implementation. Filename: `approx3D`.

Exercise 23: Use Simpson's rule and P2 elements

Redo Exercise 20, but use P2 elements and Simpson's rule based on sampling the integrands at the nodes in the reference cell. Filename: `fe_P2_simpson`.

References

[1] M. G. Larson and F. Bengzon. *The Finite Element Method: Theory, Implementation, and Applications*. Texts in Computational Science and Engineering. Springer, 2013.

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